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REDHY

Redox-Mediated economic, critical raw material free, low capex and highly efficient green hydrogen production technology

REDHY - Deliverable report

D1.2 – Data Management Plan

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Author(s)	Anna Molinari (UNR)	
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0.1	06-06-2024	UNR (Anna Molinari)	First draft
0.2	13/20-06-2024	CNR, CenMat, CNRS, IDN	Second draft
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Public Summary

The REDHy project will generate relevant amount of data related to a new highly efficient AEM technology for green hydrogen production (also at material and component level).
This includes design and production data for the components, characterization (both experimental and theoretical), but also analysis and monitoring. LCA analysis will also deliver set of data, all aimed at evaluating the proposed REDHy system performances.

The DMP presents the strategy for the data collection and generation processes during the project, including storage and management procedures, ensuring accessibility, usability, and interoperability for project partners. Additionally, it considers possible data security concerns. The DMP is in line the template provided by the European Commission and will undergo regular updates and revisions to report the data evolutions and updated details on linked management strategies. This will ensure its currency and relevance throughout the project's duration.

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1 Introduction

Report D1.2 - "Data Management Plan," is a REDHY deliverable within Task 1.4- Quality assurance and knowledge and data research management, dedicated to ensure the quality of the procedures towards obtaining reliable results in the project.

REDHy is committed to the FAIR (Findable, Accessible, Interoperable, Reusable) data framework and this document describes Data Management Plan (DMP) for the project, reporting the data to be generated, methodologies that will be used and the methods for data exploitation, sharing, accessibility, and re-use. It emphasizes that the DMP is a dynamic document, subject to updates throughout the project's duration.

The data management plan has been created with the Horizon Europe DMP template[1] and based on DLR and UNR standard management procedures and templates. The document will be update if and when necessary in order to guarantee best data monitoring procedures.

1.1 Structure of the document

The document provides at first a summary of the data that will be collected (and monitored) during the project (Chapter 2). In Chapter 3 is presented how the project will implement the Findable, Accessible, Interoperable and Reusable (FAIR) principles for data. Chapter 4 focuses on research outputs (different van data), while Chapter 5 presents the allocation of resources to implement the FAIR principles and data management as well as data security and ethical aspects. Chapter 6 and 7 describe the data security and Ethics aspects.

[1]https://ec.europa.eu/info/funding-tenders/opportunities/portal/screen/how-to-participate/reference-documents?programmePeriod=2021-2027&frameworkProgramme=43108390

2 Data Summary

The REDHy project, will generate and collect a significant amount of data across all work packages and activities. In some cases this data will be interconnected, such as the different production strategies for the System components.

The aim of REDHy, and linked data collection, is to demonstrate a new system to produce green hydrogen (WP6); this will be achieved via validation of innovative e cells design (WP5) and the necessary components (WP2,WP3 and WP4). Additionally, it aims to assess the cost, quality, sustainability, and reliability of the resulting system (WP7).

2.1 Data Types

Data generated during the project will need to be collected and monitored. To facilitate this, UNR prepared a dedicated template (short version reported in Table 2.1 and extended file in the Appendix). This template will be analysed, commented on (if necessary), and maintained during targeted discussions at Steering Committee and/or GA meetings. It is accessible to all partners and is stored in the project's shared folder on Teams.

The table and main file collect all necessary information as requested by the official template (selection in the list below):

- Data Summary
  - Type and format
  - Origin of the data
  - Quantify and storage of the data set
- Fair data
  - Naming used
  - Identifiability / Mechanism used
  - Which data will be available and how
  - Possible restrictions
  - Timing for re-use
- Allocation of resources
  - Costs
  - Responsibilities

2.2 Data Utility

Table 1 details the primary data types expected to be generated or collected within REDHY, including their purposes, production methods, formats, and potential users. The possible users cover (or should cover) the widest possible range in the sector of hydrogen production, such as the scientific community focused on advanced material production and characterization, potential end users, hydrogen producers, policy-makers, clients, and more. Additionally, the raw data sets may provide valuable information for future research. Project data also need to meet the specific needs of the REDHY partners, as outlined below. Data owners within the project are open to sharing data with other partners upon reasonable request, excluding any proprietary or sensitive company information.

Below an example of the possible REDHy data that will be generated. At the end of this report (Appendix) a more detailed table is available. The table will be updated during the entire project lifetime.

Table 2.1 Example of type of data per WP with its purpose, the data production method and format and for which user the data are useful

WP	Dataset name	Purpouse	Data Types	Origin of data	File Formats	Methods of data capture	Data Utility (for use outside consortium)
2	Theoretical calculation & design of CROC and AROC	Design of redox mediators	Modelling and Simulation	own work	raw data	Computer Simulation	
2	Characterization of CROC and AROC	Characterization	Electrochemical data, spectroscopy	own work	raw formats, excel export possible	Analytical, physical and spectroscopic characterization and measurement of electrochemical properties	
3	Bipolar Membrane Characterization	Characterization	Ex-situ, electrochemical data	own work	raw formats, excel export possible, image data (.tiff, .jpeg, etc.)	EU harmonised protocols for testing of low-temperature water electrolysers, Image data: SEM, AFM; Spectroscopic: FTIR, NMR	
4	Quantification of electron transfer kinetics in concentrated electrolytes	kinetic parameters, migration and diffusion of the redox species	Electrochemical data	own work	raw formats, excel export possible	scanning electrochemical microscopy (SECM), electroanalysis at microfibers	Limited to Consortium partners
4	Design of the porous electrode by modelling	optimize the design of REDHY electrolyzer, especially on the management of the fluidic for improved performance.	Modeling and Simulation, 3D model of porous electrode	own work	raw formats, excel export possible, image data (.tiff, .jpeg, etc.)	Computer simulation, experimental validation	Limited to Consortium partners
4	Electrode preparation with 3D printing technology and evaluation	conductivity, robustness, and flexibility of electrodes	Mechanical and thermal properties,	own work	raw formats, excel export possible	Experimental characterization	Limited to Consortium partners

5	Heterogeneous catalysts for hydrogen and oxygen evolution	activity of eterogeneous catalysts for hydrogen and oxygen evolution	Physico-chemical data, spectroscopic data	own work	raw formats, images data, excel export possible	Ex-situ validation,	
5	Single electrochemcial cell evaluation	electrochemical performance	Electrochemical data, ex-situ	own work	raw formats, excel export possible, image data (.tiff, .jpeg, etc.)	Continuous charge-discharge cycling over an extended period, monitoring any changes in capacity retention and efficiency to evaluate the degradation over time. Ex-situ characterization methods such as scanning electron microscopy (SEM) and X-ray diffraction (XRD)	
5	Prototype validation	electrochemical performance	Electrochemical data, ex-situ	own work	raw formats, excel export possible, image data (.tiff, .jpeg, etc.)	harmonised procedures for electrolyzers, TEM-EDX, SEMEDX microscopy, XPS, XRD, FT-IR	
6	Design of 5-cell stack	Stack design	Stack design	own work	CAD	Computer modelling and simulation	
6	Characterization of REDHy System	electrochemical performance	Electrochemical data	own work	raw formats, excel export possible	Testbench operation	
7	Environmental and circularity profile; Techno-economical Assessment Results	both evaluate and identify opportunities to improve the environmental and economic behavior of the REDHy technology	Life Cycle Assessment of the REDHy system, TechnoEconomical Assessment	own work	Excel, raw formats	Modelling with LCA software, own calculations based on partners' inputs. system, TechnoEconomical Assessment	Preliminary data limited to consortium partners. Conclusions and results will be made available for external stakeholders

3 FAIR data

FAIR data stands for Findable, Accessible, Interoperable and Reusable and below is reported how this principle will be applied for the REDHy project.

3.1 Making data Findable, including provision of metadata

The REDHy project and its partners will – as far as possible – allow all data generated and collected within the project to be easily findable. This will be done by providing the related set of metadata describing the dataset with a standard and unique identifier.

In case of scientific publications the Digital Object Identifier (DOI) will be provided, while all deliverables (and other project reports) that are intended for public use will also be made available for download via the project website.

The basic metadata that will be defined for each dataset (or document) are the following:

- Title
- Description
- Creator and contributors
- Specification of the data identifier(s)
- Publisher (if relevant)
- Date of data collection
- Dates of document creation and last revision
- Language
- Keywords (defined by partners)
- Acknowledgement of the Clean Hydrogen and EC funding of the REDHy project

In order to guarantee an easy and fast identification and indexing, the consistent naming of all the data will function as metadata. In example, the following coding is suggested for project deliverables:

REDHy_<dnum>_<dname>_<sdis>_<ver>_<orgshortname>.pdf

- <dnum> represents the code of the deliverable
- <dname> the name of the deliverable as stated in the DoA
- <sdis> is filled with the acronyms related to dissemination level (e.g. co = confidential, pu = public) **- Optional**
- <ver> the version of the document.
- <orgshortname> organization that is performing the changes on the version

Version 1.x will indicate that the document is still a draft. Further revisions or new issues of a deliverable will make use of the following format: v2.x. The official document to be sent to the Clean Hydrogen and European Commission (EC) will be labelled as 'Final'. In case of necessary revisions requested by the EC, the report will be labelled as: Revision1, Revision2….

Summarising: Data will be preserved in open, or restricted, repositories as appropriate and obtain a DOI. Metadata will follow standards set by the field. Should there be no relevant field standards, the consortium will create their own metadata standards and keep documentation.

3.2 Making data Accessible

The principle to have data "as open as possible, as closed as necessary" will be applied for the REDHy project. The project is a research and innovation action, meaning there may be many data generated which will be considered as confidential (i.e., relevant to the producing partner for possible patenting or publications).
Access limitation to public data and possible embargo periods will be defined at the time it is needed due to IPR or confidentiality issues.

Nevertheless, the project foreseen Public Deliverables (those deliverables classified as PU), which data will be made openly available. Such deliverables will be shared via the project website and via partners' own repository. If specific instructions are needed to facilitate data access, such as details regarding the nature and origin of the data, these will be provided when the data is deposited. Data selected for open access will be made available without restrictions. Data related to 'SEN' Deliverables (confidential and classified) at the consortium level will be stored on the internal project platform (Teams) with access restricted to consortium partners.
Metadata will be made openly available and licensed under a public domain dedication, as per the grant agreement, unless it is against a beneficiary's legitimate interests, including exploitation or contrary to other constraints like the EU competitive interests or obligations under the GA. The possible update of DMP will list any exceptions to the public domain dedication.
Partners used repositories are: ZENODO, SOLAR, and own-institute repository

In the case of research data, data will be preserved for a minimum of 10 years at each project partner on local servers The coordinator (DLR) will store all relevant data in addition to the research data for 10 years. Research data will also made available along with publications if this is foreseen by the target journal.

3.3 Making data Interoperable

To guarantee data interoperability, REDHy project data, including metadata, will be standardized using a formal, accessible language. The interoperability of data and research outputs will be maintained by using standard processing software where possible (e.g., Windows Office, PDF). If cross-references to data are necessary, such as the production and evaluation of performance for particular material or components, qualified references will be provided as far as possible.

Partners will arrange access to specialist software (e.g., modelling, data processing, or software for specific test methods) on a bilateral or project-wide basis, depending on need and license availability. All data collected during the project will be exported to standard data formats whenever possible to facilitate interoperability. These formats may include .rtf, .txt, and .docx for reports, and .csv and .xlsx for numerical datasets. Although .docx and .xlsx formats are specific to Microsoft Office and not universally standard, they are included due to the widespread use of Microsoft Office.

3.4 Increase data Re-use

REDHy has no standard (yet) - at this stage of the start of the project - regarding the licensing of data generated and (most likely) data licensing will be decided on a case-by-case basis. Whenever feasible, the most open approach recommended by Clean Hydrogen/Horizon Europe guideline will be employed, except for data deemed commercially confidential, which will be subject to more restrictive licensing. Any instances where data licensing is required will be documented in a forthcoming update to the Data Management Plan (DMP).
In principle, data will remain usable, i.e., not outdated, for a period of 10 years following the completion of the project.

Long term preservation of restricted or closed data will be ensured by the partner that created the data. It is foreseen that many partners will use Zenodo, or similar platforms, to store restricted and open data. Open/ Public data will be also kept via the project website, which will be updated till project ends and maintained 'on air' up to 2 years after the project.
Management of partner-own data after the project will be responsibility of the data-owner.
Restricted and closed data will be added to the partner-data repository where it will be stored cost-free for a minimum of 10 years.

In the possible updates of the DMP partners will provide plans for how the long-term preservation of the closed and restricted data they created will be ensured.

4 Other research outputs

REDHy has an internal process for quality management and monitoring that is active throughout the entire project duration. This task (Task 1.4) covers the quality assessment of both project data/products and project processes (refer to D1.1 Quality Management and Knowledge management Plan). Results, not limited to data, will also be analysed and collected throughout the project. To this end, the Communication and Dissemination Plan (D8.2- Plan for DEC activities) is being prepared and will be updated by each partner at each reporting period or more frequently if necessary.

All project results, including research data, publications, product information, policy discussions, will be analysed and documented using the Data Inventory Table (Appendix). WP leaders and partners responsible for publications are required to periodically fill in this table. Updates to the Data Management Plan will include revisions to the online repository where information is collected and shared.

5 Allocation of resources

The primary responsibility for data management lies with the principal investigator at each project partner. Storing project data, such as in the European Open Science Cloud[2] (EOSC), OpenAIRE[3] , Registry of Open Access Repositories[4] (ROAR), and Directory of Open Access Repositories[5] (OpenDOAR), is free of charge. However, allocating person-months will be necessary to prepare the files for storage. Personnel costs associated with data handling efforts are accounted for within the project's budget.

The potential values linked to the long-term preservation of data, as well as associated costs will be discussed among the consortium if necessary in the coming months. This includes considerations on how data will be retained beyond the project's duration, for a minimum of 2 and up to 10 years, and how these costs will be covered and by whom.

5.1 IPR Protection Strategy

The focus within the REDHy project is on tackling the limitations of contemporary electrolyser technologies by fundamentally reimagining water electrolysis, allowing it to surpass the drawbacks of state-of-the-art (SoA) electrolysers and become a pivotal technology in the hydrogen economy.
The project approach will be highly adaptable, enduring, environmentally friendly, intrinsically secure, and cost-efficient, enabling the production of economically viable green hydrogen at considerably increased current densities compared to SoA electrolysers.
This will have as potential outcome the generation of new Intellectual Property (IP) for partners (maybe even new patents). Access to this IP will be provided to partners as appropriate, in line with the Consortium Agreement. Management of Open Science Practices and Intellectual Property Rights (IPR) protection activities will fall under WP1 and WP8.

The project's IPR strategy (which will be outlined in D8.2 and D8.3) aims to enable partners to strengthen their market position through patent protection. Partners signed a Consortium Agreement outlining rules for confidentiality, ownership, and IPR issues. This includes details on procedures for granting publication of results, ownership regimes, and IPR matters such as background and excluded ownership, licensing terms, etc

[2] About | EOSC Portal (eosc-portal.eu)
[3] OpenAIRE
[4] Welcome to the Registry of Open Access Repositories - Registry of Open Access Repositories (eprints.org)
[5] Welcome to OpenDOAR -

6 Data Security

Project data will be stored in project's and partners' repositories to enhance accessibility to a broader community, categorized as follows:

- **Public:** This category includes project data that can be openly published on the project website or registries of scientific repositories, making it accessible to a wider audience.
- **Confidential:** Data in this category are subject to obligations to third parties, prohibiting full disclosure. Therefore, dissemination to the public will occur only with the agreement of project partners and in a restricted manner. Deliverables labelled as "confidential" in terms of dissemination level and listed as such in the Grant Agreement fall under this classification.
- **Internal:** This category encompasses project raw data utilized exclusively by consortium partners during the project, not intended for public dissemination.

Each consortium partner bears the responsibility for appropriately storing, processing, and sharing the data generated during their project activities. Additionally, partners are accountable for ensuring sufficient storage capacities, data backup, and recovery in accordance with their organization's internal policies.

7 Ethics

Regarding ethical considerations, no issues have been identified or are anticipated to arise from the research activities of REDHy that could impede data sharing.

8 Other Issues

An appropriate Consortium Agreement has been established to govern the ownership of results and access to critical knowledge, including Intellectual Property Rights (IPR) and research data. The IPR strategy covers various commercialization avenues such as patents, copyrights, and trade secrets, in alignment with general EC policies on ownership, exploitation rights, confidentiality, commercial utilization of results, and availability of information and deliverables (refer to chapter 5.1).

Critical Intellectual Property (IP) necessary for the successful execution of the REDHy project is either owned by consortium members or has undergone preliminary freedom-to-operate checks, with IPR protection measures detailed in the Consortium Agreement. Background IP contributed by partners will remain accessible for use and will remain the property of the original owner. IP generated during the project will be owned by the partner(s) responsible for its development.

Decisions regarding the publication of IP will be made jointly by the consortium partners, while the strategy for exploiting results will be determined on a case-by-case basis, ranging from open access to licensing arrangements.

9 Conclusion and Recommendations

This deliverable report provides an initial outline of the Data Management Plan (DMP) for the REDHy project, detailing the generation, handling, preservation, and re-use of research data. Additionally, methods demonstrating how to ensure data are Findable, Accessible, Interoperable, and Reusable (FAIR) are presented. The consortium is committed to adhere to the provisions outlined in this report.

It's important to highlight that this document is dynamic and subject to modifications and updates throughout the duration of the project.

10 Risks and interconnections

10.1 Risks/problems encountered

No risks arisen related to this deliverable. This is a living document, which will be monitored and updated throughout the project lifetime.

10.2 Interconnections with other deliverables

This Data Management Plan also describes data that will lead to results that might have possible exploitable value. Therefore, this DMP can also be seen as making clear, which partner(s) will produce particular data for possible future exploitation and intellectual property protection. Since the Deliverable on the final Exploitation Plan later in the project (M12), the DMP serves as the initial guidance for these exploitations.

11 Acknowledgement

The author(s) would like to thank the partners in the project for their valuable comments on previous drafts and for performing the review.

Project partners:

#	Partner short name	Partner Full Name
1	DLR	DEUTSCHES ZENTRUM FUR LUFT – UND RAUMFARHT EV
2	CNRS	CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE
3	UNR	UNIRESEARCH BV
4	UPV	UNIVERSITAT POLITECNICA DE VALANCIA
5	IDN	INDUSTRIE DE NORA SPA-IDN
6	CENMAT	CUTTING-EDGE NANOMATERIALS CENMAT UG HAFTUNGSBESCHRÄANKT
7	CNR	CONSIGLIO NAZIONALE DELLE RICERCHE

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Appendix – DATA INVENTORY Table

Dataset name	WP	Partner Responsible	Purpouse	Open Restricted	Data Types	Origin of data	New/Existing Data	File Formats	Methods of data capture	Size	Storage of data	Data Utility (for use outside consortium)	Type of IP	How will be re-used	Timing for re-use	Ethical/ Issues (Y/N)
3D electrode model	4	CNRS	Design of electrode flow path	Open	Graphical	Laboratory experiments	New	.stl, .f3d.	Fusion360, CAD software	50 MB	Lab computer + PETA	Limited to consortium partners	_	Printed in other ink materials	5 years	N
Ink rheology	4	CNRS	Characterization of rheological propierties of inks	Open	numerical dataset	Laboratory experiments	New	.txt	TA instruments AR2000 rheometer	50 MB	Lab computer + PETA	Limited to consortium partners	_	Comparison studies	5 years	N
Multiphysics simulations	4	CNRS	optimization of the electrochemical, fluidynamics and thermal behaviour of the electrode system.	Open	numerical dataset	Laboratory simulation	New	.mph, .txt	COMSOL	50 GB	Lab computer + PETA	Limited to consortium partners	_	Tool for improving electrode design	5 years	N
3D Electrode	4	CNRS	Electrode prototyping	open	Physical object	Laboratory experiements	New	physical object	DIW printer	according to electrochemical systems	Lab computer + PETA	Limited to consortium partners	_	Tested in other electrolytes	5 years	N
Electrochemical behaviour	4	CNRS	Electrochemical characterization of the electrode material, optimization of multiphysics simulations	open	numerical dataset	Laboratory experiments	New	.mps .txt	Biologic Electrochemical workstation	500 MB	Lab computer + PETA	Limited to consortium partners	_	Comparison studies	5 years	N
SEM/EDS	4	CNRS	Physical characterization of electrode/inks	open	optical images	Laboratory experiments	New	.jpg, .txt	JEOL IT 500 HR	50 MB	Lab computer + PETA	Limited to consortium partners	_	_	5 years	N
Mechanical testing	4	CNRS	Physical characterization of electrode	open	numerical dataset	Laboratory	New	.txt	Femto Tools Station/	10 MB	Lab computer + PETA	Limited to consortium partners	_	Comparison studies	5 years	N

			(conductivity, flexibility, robustness)			experiments			Universal testing Machine							
Spectroscopy characterization	4	CNRS	Physical characterization of electrode/inks	open	numerical dataset	Laboratory experiments	New	.txt	Instruments of the SMI platform at LCPME	50 MB	Lab computer + PETA	Limited to consortium partners	_	_	5 years	N
ink formulation	4	CNRS	Composition of inks	restricted	text, numerical	Laboratory experiments	New		Manual entry	5 MB	Lab computer + PETA	Limited to consortium partners	secret or patent	_	5 years	N
Printing protocol	4	CNRS	Documentation of steps and parameters for a successfull print	restricted	text, numerical	Laboratory experiments	New	.xlsx, .docx	Manual entry	5 MB	Lab computer + PETA	Limited to consortium partners	secret or patent	_	5 years	N
Theoretical calculation & design of CROC and AROC	2	UPV	Design of redox mediators	Restricted	Modelling and Simulation	own work	New	raw data	Computer Simulation							
Characterization of CROC and AROC	2	UPV	Characterization	Restricted	Electrochemical data, spectroscopy	own work	New	raw formats, excel export possible	Analytical, physical and spectroscopic characterization and measurement of the electrochemical properties							
Bipolar Membrane Characterization	3	CENMAT	Characterization	Restricted	Ex-situ, electrochemical data	own work	New	raw formats, excel export possible, image data (.tiff, .jpeg, etc.)	EU harmonised protocols for testing of low-temperature water electrolysers, Image data: SEM, AFM;	50 MB	Online Drive	Limited to consortium partners		Comparison studies		N

								Spectroscopic: FTIR, NMR							
Quantification of electron transfer kinetics in concentrated electrolytes	4	CNRS	kinetic parameters, migration and diffusion of the redox species	Restricted	Electrochemical data	own work	New	raw formats, excel export possible	scanning electrochemical microscopy (SECM), electroanalysis at microfibers						
Design of the porous electrode by modelling	4	CNRS	optimize the design of REDHY electrolyzer, especially on the management of the fluidic for improved performance.	Restricted	Machine data, 3D model of porous electrode	own work	New	raw formats, excel export possible, image data (.tiff, .jpeg, etc.)	Computer simulation, experimental validation						
Heterogeneous catalysts for hydrogen and oxygen evolution	5	CNR	activity of eterogeneous catalysts for hydrogen and oxygen evolution	Restricted	Physico-chemical data, spectroscopic data	own work	New	raw formats, images data, excel export possible	Ex-situ validation,						
Single electrochemcial cell evaluation	5	CNR	electrochemical performance	Restricted	Electrochemical data, ex-situ	own work	New	raw formats, excel export possible, image data (.tiff, .jpeg, etc.)	Continuous charge-discharge cycling over an extended period, monitoring any changes in capacity retention and efficiency to evaluate the degradation over time. Ex-situ characterization methods such as						

								scanning electron microscopy (SEM) and X-ray diffraction (XRD)								
Prototype validation	5	CNR	electrochemical performance	Restricted	Electrochemical data, ex-situ	own work	New	raw formats, excel export possible, image data (.tiff, .jpeg, etc.)	harmonised procedures for electrolyzers, TEM-EDX, SEMEDX microscopy, XPS, XRD, FT-IR							
Design of 5-cell stack	6	DLR	Stack design	Restricted	Stack design	own work	New	CAD	Computer modelling and simulation							
Characterization of REDHy System	6	DLR	electrochemical performance	Restricted	Electrochemical data	own work	New	raw formats, excel export possible	Testbench operation							
Environmental and circularity profile; Techno-economical Assessment Results	7	IDN	both evaluate and identify opportunities to improve the environmental and economix behavior of the REDHy technology	Restricted	Life Cycle Assessment of the REDHy system, TechnoEconomical Assessment	own work	New	Excel, raw formats	Modelling with LCA software, own calculations based on partners' inputs. system, TechnoEconomical Assessment		few MB	Preliminary data limited to consortium partners. Conclusions and results will be made available for external stakeholders	Not applicable	Comparison studies	Not applicable	N