Deliverable report

D7.9 Data Management Plan

WP7 – Communication, dissemination and exploitation

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Name	Organisation	Role	Action	Date
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Joris Thybaut	Coordinator	UGent	22/03/23	ok

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To request a change to this document, contact the Document Author.

CONFIGURATION MANAGEMENT

Nature of Deliverable		
R	Document, report (excluding the periodic and final reports)	
DEC	Websites, patents filing, press & media actions, videos, etc.	
DEM	Demonstrator, pilot, prototype, plan designs	
OTHER	Software, technical diagram, algorithms, models, etc.	
ETHICS	Deliverables related to ethics issues.	
DATA	Data sets, microdata, etc	
DMP	Data Management Plan	X

DISSEMINATION LEVEL		
PU	Public, fully open, e.g., web (Deliverables flagged as public will be automatically published in CORDIS projects.)	X
SEN	Sensitive, limited under the conditions of the Grant Agreement	

ACRONYM/ABBREVIATIONS	
CA	Consortium Agreement (contractual document between members of the consortium)
DoA	Description of Action (technical annex to the Grant Agreement)
EC	European Commission
EU	European Union
FTP	Funding and Tenders Portal: https://ec.europa.eu/info/funding-tenders/opportunities/portal/screen/home
GA	Grant Agreement (contractual document between EC and beneficiaries)
IPR	Intellectual Property Rights
KO	Kick Off (meeting)
MC	Management Coordinator
MTA	Milestones Trend Analysis
N/A	Not applicable
PC	Project Coordinator
PMO	Project Management Office
TL	Task Leaders
WP	Work Package
WPL	Work Package Leaders

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Contents

1 EXECUTIVE SUMMARY

1.1 Description of the deliverable content and purpose

This is the first version of the e-CODUCT Data Management Plan (DMP). The DMP is a living document that describes the data we expect to acquire or generate during the course of e-CODUCT, how we will manage, describe, analyze, and store those data, and what mechanisms we will use at the end of the project to share and preserve the data.

1.2 Corrective action vs. Grant Agreement (if relevant)

The deliverable is submitted within 1 month after the initial due date, without impacting the critical path of the project. Indeed the content was discussed during the 6-Month meeting of the project with all partners (15&16th of March 2023).

2 DESCRIPTION OF THE DELIVERABLE OBJECTIVE AND CONTENT

This document describes the Data Management Plan (DMP) that will be used within the 'Fast-response Electrically heated catalytic reactor technology for CO_2 reDUCTion' (e-CODUCT) project, funded by the EU. DMPs are a crucial component of effective data management. They outline the life cycle of data that will be collected, processed and generated within a project, here a Horizon Europe project, with the goal of making research data findable, accessible, interoperable, and reusable (FAIR). This DMP provides guidance for the e-CODUCT consortium on how to effectively and validly collect, store, use, and dispose of data throughout the project.

This document describes the types of data that will be collected, the sources and purposes of the data, and the conventions and restrictions for naming, storing, and sharing the data. It also explains the FAIR data management principles and how they will be applied in the e-CODUCT project, and addresses resource allocation, data security, and ethical considerations for data collection and use.

During the project several types of data will be generated which are identified by this DMP and rules for its management covering data sharing, disclosure and security in line with Horizon Europe rules for fair data management as set out in the Guidelines on FAIR Data Management in Horizon Europe are established.

The DMP serves as a living document that will be reviewed and updated at each project meeting, in accordance with Horizon Europe guidelines on FAIR data management. This document was created with the assistance of the Data Steward Team of UGent.

The provisions for open access to research data are described in the Grant Agreement.

3 DATA SUMMARY

3.1 Purpose of data collection/generation and relation to the objectives of the project

The e-CODUCT project aims at the simultaneous reduction of CO_2 and H_2S into a platform molecule (CO) and a marketable product (S_X), which is an ongoing challenge in the field of carbon capture, as no existing technologies are able to accomplish this. Within this project, a novel strategy will be developed for two-step acid gas valorization via i) conversion of CO_2 and H_2S into COS in a fixed bed reactor, and ii) COS conversion into CO and S_X using an electrothermal fluidized bed (ETFB) reactor. At the end of the project, a working pilot plant is envisaged. Nine beneficiaries are working together in a multidisciplinary manner to achieve this goal, namely:

1. UNIVERSITEIT GENT (UGent)
2. TOTALENERGIES ONE TECH BELGIUM (TOTB)
3. KEMIJSKI INSTITUT / NATIONAL INSTITUTE OF CHEMISTRY (NIC)
4. PDC RESEARCH FOUNDATION (PDC)
5. CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE CNRS (CNRS-LCS)
6. SAINT-GOBAIN CENTRE DE RECHERCHES ET D'ETUDES EUROPEEN (SG CREE)
7. DECHEMA GESELLSCHAFT FUR CHEMISCHETECHNIK UND BIOTECHNOLOGIE (DECHEMA)
8. BENKEI (Benkei)
9. CENTER ODLICNOSTI NIZKOOGLJICNE TEHNOLOGIJE ZAVOD (CO NOT)

The purpose of data collection is strongly linked with the objectives, the planned activities and outcomes of e-CODUCT, which are:

OBJECTIVE 1: Demonstrate pilot scale conversion of CO_2 and H_2S into COS

OBJECTIVE 2: Demonstrate ETFB technology for conversion of COS into CO

OBJECTIVE 3: Validate reaction products quality and valorize CO by conversion into green methanol

OBJECTIVE 4: Construct reactor and process models with integrated microkinetics for process optimisation and scale-up

OBJECTIVE 5: Demonstrate techno-economic and environmental performance of reactors and models

3.2 Types of data generated and collected

The table below gives a preliminary outline of the data which will be generated and collected throughout the project, grouped by beneficiary and provided with the following information:

- Data types, e.g., spreadsheets, text, images, samples, models
- Source of data, e.g., experiments, databases, simulations
- Formats of data, e.g., .csv, .xlsx, .docx, .pdf, .txt, .jpg
- Expected size of data
- How and where the data and backups will be stored?
- Is the data public, internal, restricted or confidential?
- How will the data be disseminated or published?

Beneficiary	Data types and their Sources	Formats	Size	Storage	Confidentiality	Dissemination/ Publishing
UGent	Models will be developed based upon experimental data generated by NIC and SG CREE as well as on data openly available in literature. The models will be used to generate novel data (spreadsheets) by means of simulations.	.mlx .csv	Below 1GB	All developed software and generated modelling data will be stored for at least 20 years in the software and data library of LCT-UGent.	The models are considered restricted, but can be used by third parties through licensing. The data generated using the models are considered public.	The insights obtained from the models will be published in high impact journals. After publication of said papers, the corresponding modelling data will be openly deposited in Zenodo.
TOTB	Literature, market data for compounds, information about and from production sites. Analysis of pilot operation parameters and industrial suitability.	.xlsx .docx .pptx .pdf	Below 1GB	Private SharePoint server with controlled access.	The data on market analysis and data from sites is restricted. Processed data with business case will be shared within the consortium. Pilot operation data is partially restricted.	Business case analysis will be disseminated within the consortium and in censored (reduced) version – in public. Pilot operation data will be disseminated through e-CODUCT web page in censored (reduced) version, agreed with consortium members. The process data will be openly deposited in Zenodo.
NIC	1. Collecting of COS decomposition reaction kinetics data (laboratory experiments). 2. Design of the project identity (logos, videos, web page)	.pdf .xls .jpg .png .mp4 .avi	Below 1GB	Data are stored in the NIC data storage system and backed up.	Majority of the data are considered public	Experimental results will be published in high impact journals. After publication of said papers, the corresponding data will be openly deposited in Zenodo. The project identity is a part of the public dissemination plan. Web page www.e-coduct.eu is publicly available, video is uploaded to the e-CODUCT social media.

PDC	1. Process balance models and stream tables will be developed in MS Excel, as well as technoeconomic analysis. 2. Detailed process simulations done in ASPEN Plus software (licensed).	.pdf .xlsx .xlsm .docx .apwz .bkp	Below 1 GB	Data is stored on PDC internal servers with several backup modules.	The models and simulations are confidential to the consortium. The results derived from them might be, however, used in publications and other works.	Dissemination of the data is directly linked to the deliverables listed in the GA. Main model and simulation results can be used for the purposes of public communication and academic publications by other members of the consortium.
CNRS-LCS	Zeolite samples will be prepared and subjected to physicochemical characterizations. The zeolite samples will be tested in the reaction H2S + CO2.	.pdf .xlsx .docx .ppt .org .chrx	Below 5 GB	Data is stored on the computer connected to the setup. We plan to store the data on the LCS internal server as well.	The majority of the data is considered public. Detailed elements are confidential to the partners.	Experimental results will be published in high impact journals. After publication of said papers, the corresponding data will be openly deposited in Zenodo.
SG CREE	Samples will be generated and analyzed and tested.	.pdf .xls .docx .ppt .jpg .png .mov	Below 1GB	Data is stored on Saint-Gobain storage system and backed up.	Data is confidential to the consortium. Detailed elements are confidential to the partners.	Some of the data may be disseminated through patenting if relevant. After filing the patent, the corresponding data will be openly deposited in Zenodo.
DECHEMA	1. typical data types for general data and image creation/transfer. Possibly also .svg for easier zooming into images. 2. Simulations in Aspen Plus, saved as .apwz or bkp. Simulations in Aveva is saved in .simx	.pdf .xlsx .docx .ppt .jpg .png .svg .apwz	Below 1GB	Simulations are mostly saved on our system. We also have a backup system on DECHEMA side. Some files will be shared with partners	The models and simulations are mostly confidential to the consortium. The results and learnings could be public.	Dissemination of the data is directly linked to the deliverables listed in the GA. Depending on results and learnings some could be published as a paper in a journal. After publication of said papers, the corresponding data will be openly deposited in Zenodo.

		.bkp .simx		working in the same WPs.		
Benkei	Financial (efforts and expenses) data for management and reporting purposes	.xls .pdf	Below 1GB	Sharepoint (common repository platform), EU F&T portal	Data is confidential to the consortium. Detailed elements are confidential to the partners.	Neither dissemination nor publishing outside the consortium and EU.
CO NOT	1. Technical documentation for the ETFB reactor fabrication – CAD drawings of the reactor and its components, bill of materials. 2. Mathematical modeling and CFD simulations of the reactor.	.sldprt .sldasm .pdf .xls	Below 1GB	Data are stored in the CO NOT and NIC data storage system and are backed up.	Some data are confidential to the consortium. Final results of the reactor operation are considered public.	The reactor itself and the results of COS decomposition in ETFB reactor will be published in high impact journals. After publication of said papers, the corresponding data will be openly deposited in Zenodo.

4 FAIR DATA

4.1 Making data findable (F)

4.1.1 Repository and Persistent identifiers (PID)

The e-CODUCT project is committed to the principle of open access to research data. Hence, all data that can be made publicly available will be archived in the Zenodo repository. Zenodo is a free online archive created by CERN and the EU OpenAire project. It provides a storage capacity of 50 GB per dataset and guarantees preservation for at least 20 years. It also assigns a unique and persistent identifier, typically in the form of a DOI, which makes it easy to retrieve and cite the data. This ensures that the data generated by the project will remain accessible to the research community for an extended period.

Researchers involved in the e-CODUCT project are encouraged to create an Open Researcher Contributor ID (ORCID), which is a widely recognized standard and service that helps researchers establish and maintain their research identity, minimizing name confusion.

4.1.2 Metadata

Each dataset produced will be described using standardized metadata, which facilitates efficient data sharing among researchers. As a general rule, the e-CODUCT will use the DataCite Metadata Schema, which is compatible with the OpenAIRE platform and the project's use of Zenodo.

The metadata for each dataset will contain information that is relevant to the nature of the data and will include information such as creator, access conditions, experimental methods, time references, data file organization and structure, file formats, variable names, etc. Thematic keywords will also be provided to enable other researchers to easily understand the context and background of the data, making it more valuable for reuse.

4.1.3 Naming conventions and versioning

The e-CODUCT project has established a consistent naming convention for all project files to ensure that they can be straightforwardly organized and identified. The naming convention adopted is as follows: **'date (yyyymmdd)_e-CODUCT_title_version'**. This format includes the date the file was created, the e-CODUCT project, a title that describes the content of the file, and version number. Any changes made to the dataset after deposition will be logged in the version control system of the repository.

4.2 Making data openly accessible (A)

4.2.1 Confidentiality

There are four levels of data confidentiality considered in this DMP:

- **Public:** the data can be made public (openly available), although in most cases this will only be after the publication of the corresponding manuscript;
- **Internal:** the data is shared only between project partners and cannot be made public during or after the project;
- **Restricted:** access is restricted due to an embargo period or only certain project partners can access it;
- **Confidential:** the data is only accessible by people linked to a certain beneficiary.

The level of confidentiality will of course depend on the data generated, but an indication of what is expected is already listed in the table above. Confidential or restricted data are expected to be mainly company related and, in such cases the confidentiality will be governed by specific partner agreements.

4.2.2 Data repository

As mentioned in section 4.1.1, public data and corresponding metadata will be deposited in a certified data repository, which provides a support structure for data preservation and sharing, as well as safe and sustainable data storage facilities. As a general rule, project partners will use the Zenodo data archive (https://zenodo.org/) as the primary repository for depositing data. Upon deposition, the data supplier and repository will sign an archiving agreement that outlines the terms and conditions for data archiving and access. After the end of the project, and as soon as project results have been published in the form of peer-reviewed publications, the e-CODUCT consortium will strive to make as much as possible Internal, Restricted and Confidential data Public. In cases where full open access to the data is not possible due to confidentiality concerns as outlined above, metadata will be made available.

4.2.3 Website

Links to all datasets which were made publicly available in the data repository, as well as to all peer-reviewed publications resulting from this project, will be provided at the e-CODUCT website.

4.3 Making data interoperable (I)

Data exchange and reuse by other researchers will be facilitated by depositing and archiving the data in standard formats that are compatible with commonly used open-source software. Appropriate file formats for different types of data have been identified and are listed in the table above. The file formats for the different kinds of data are equally listed in the table. Standard vocabulary and terminology will be used to ensure interdisciplinary interoperability.

4.4 Making data re-useable (R)

All data that can be made public will be released via Creative Commons license CC-BY or CC-0, in compliance with EU guidelines. Data that have been classified as Public will be made available on the Zenodo platform immediately after upload. In principle, all data will be re-usable by third parties, unless special restrictions apply which will be indicated in the accompanying metadata.txt file. It is intended

that the data remain reusable for at least 20 years, allowing it to remain valuable to the research community long after the project's completion.

5 ALLOCATION OF RESOURCES

5.1 Costs

The costs associated with data management on the level of the individual researchers, i.e. short-term data storage, will be covered by the project beneficiaries. Costs related to data generated or acquired on the e-CODUCT management level are covered by Benkei. Long-term preservation of data will not incur additional costs, as archiving in the Zenodo repository is offered free of charge.

5.2 Project responsibilities

Data management is part of WP7 of which the lead beneficiary is NIC. However, the task of the establishment and development of the DMP is the responsibility of UGent. The e-CODUCT Supervisory Board is responsible for elaborating and adopting the DMP, as well as informing the individual researchers and overseeing that the requirements are met and deadlines respected. Each researcher is responsible for creating an individual data management plan, and for handling the research data in line with the provisions of the e-CODUCT DMP.

6 DATA SECURITY

Within the organizations of each of the beneficiaries, there are systems in place to ensure the secure storage and preservation of all data collected and generated throughout the project. Throughout the project, in the data gathering and analyzing phase, individual researchers will store data in their personal password-protected spaces on secure university servers, which provide appropriate back-up solutions. Files related to project management and progress meetings will be stored on a dedicated Sharepoint, hosted by Benkei, which is equipped with appropriate back-up solutions as well. The data which can be made public will be deposited for long-term storage in certified repositories, such as the Zenodo data archive, which are again equipped with backup systems.

7 ETHICAL ASPECTS

Within this project no personal data or data that could be ethically sensitive will be collected.