Ref. Ares(2021)2507555 - 13/04/2021

SCARABEUS

H2020 Research and Innovation Action project, Grant Agreement number 814985

D7.9 – Final Data Management Plan

This Deliverable 7.9 report is part of a project than has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 814985

WP 7: Dissemination, Communication and Exploitation

Task 7.3: Exploitation

Version: Revised final version, April 13th 2021

Technical References

Deliverable No.	7.9 - Final Data Management Plan
Dissemination level [1]	Public
Work Package	7 - Dissemination, Communication and Exploitation
Task	7.3 - Exploitation
Lead beneficiary	Abengoa Energia
Contributing beneficiary(ies)	USE, POLIMI
Due date of deliverable	March 30th 2021 (M24)
Actual submission date	April 13th 2021

[1]PU = Public
PP = Restricted to other programme participants (including the Commission Services)
RE = Restricted to a group specified by the consortium (including the Commission Services)
CO = Confidential, only for members of the consortium (including the Commission Services)

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History of Changes

Version	Date	Changes
#1	11/02/2021	Original version created by Antón López
#2	29/03/2021	Version sent to the Coordinator
#final	13/04/2021	Final version approved by Giampaolo Manzolini

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Executive Summary

This document describes the main features of the data repository: the folder structure for the data server, the access rights, the data management responsibilities and the coding expected for certain documents. The security of the system to guarantee the safety of the information is also described. Finally, the type of results included in the Open Data Pilot are described together with the timing.

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Nomenclature/Acronyms

WP: Work Package
POLIMI: Politecnico di Milano
TUW: Technische Universitaet Wien
KELVION: Kelvion Thermal Solutions
EXERGY: Exergy SPA
USE: Universidad de Sevilla
CITY: City Univesity of London
QUANTIS: Quantis
ABENGOA: Abengoa Energia
UNIBS: Universita degli studi di Brescia

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Introduction

For the proper operation of the consortium members, the SCARABEUS project implements a data repository available for all members. The structure and management of that repository is outlined in this document.

This data repository has two main objectives:

- To serve as a communication tool among the Project Consortium for distributing information
- To store all relevant information (internal and official reports, reports on deliverables, relevant documents and results, etc.), so they are always available for every partner through internet access

This document serves as a guideline to ensure the correct use of the data repository, what implies being respectful with the agreed internal structure of folders and subfolders and with the standardization of folder/file names. The information that is necessary to adjust to these rules for the correct management of data is provided in this document.

In addition, the SCARABEUS project applied to the Open data PILOT. To implement such plan, section 8 of this document presents the roadmap to be followed by the consortium members to ensure that the project results and data are adequately shared with the scientific and industrial communities. The key persons responsible for the implementation are also reported.

Data repository

All the relevant data has to be available to the interested partners. To accomplish this operational objective effectively, reliably and seamlessly, the file-exchange system is implemented in an internet server system, hence ensuring that all partners with an internet connection have instant access to the results provided by their colleagues, thereby reducing delays and enhancing the flow of information.

1 Physical location

The server is implemented in the cloud and managed by University of Seville along with the project website. This join management of the web and repository has multiple benefits:

- Lower cost of common services.

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- Faster feedback from webmaster and supervisor of the repository (single hub for communications regarding both tools).
- Standardization of communication protocols.

2 Backup and security

Data in the repository is stored and organized in a MySQL-type database managed by a server running on GNU-Linux operating system. These data will be secured through disk backups performed daily from Monday to Saturday. These backups are acknowledged to be secure and cost-effective and they store both the files uploaded in the repository (database) at any point in time and also the settings of the GNU-Linux server. Security of the data stored in the server will be ensured through appropriate firewalls and multiple filter software preventing all sort of attacks to the server and users: Fail2ban (intrusion prevention software protecting servers from massive -brute-force- attacks), SpamAssasin (software filtering spam email), SPF/DKIM filter (software to prevent phishing), geographic identification of users to detect fraud, 24/7 lookup and surveillance through software such as nagios/nrpe and others.

3 Accessibility

All the data stored in the data repository is for members only. The access will be protected by username and password, each user having a unique identifier. All members of any organization will have their own username and password, granting different access rights depending on the access matrix (defined in 5. Access rights)

4 Data folder tree

A folder tree (structure) is defined in order to organize all the information in the repository. This structure can be modified under a reasoned request by any consortium member, addressed to the Dissemination Manager. The DM will then share the suggestion with the Consortium Partners who will eventually agree with the interested party on an appropriate modification of the structure. In case of conflict, or if the requested modification can be considered major, the Dissemination Manager will forward the request to the Project Coordinator for further discussion and decision making by the Project Management Team.

The folder tree is defined as follows:

General Info folder:
Contractual documents folder
Grant Agreement
Consortium Agreement

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Amendments
Dissemination templates folder
Templates
Dissemination and Communication Plan (with supporting documents)
Logos folder
List of participants and contact info (email and telephone number)
List of WP leaders
List of other relevant positions (Risk Manager, Dissemination Manager, Project Coordinator…)
Updated Gantt chart

Work Package folder:
WP1 folder: Contain information relevant for WP1 members
WP2 folder: Contain information relevant for WP2 members
WP3 folder: Contain information relevant for WP3 members
WP4 folder: Contain information relevant for WP4 members
WP5 folder: Contain information relevant for WP5 members
WP6 folder: Contain information relevant for WP6 members
WP7 folder: Contain information relevant for WP7 members
WP8 folder: Contain information relevant for WP8 members

Deliverables folder

Financial

Meetings folder:
One subfolder for each meeting
Minutes of the meeting
Agenda and useful information
WP presentations
Pictures

Image folder

File – exchange folder:
Subfolders upon request

Publications folder:
All publications related to the SCARABEUS project should be uploaded into this folder
Journal articles
Conference proceedings
Other publications

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5 Access Rights

The following user categories, with different access rights, are defined:

- **Group A**: Administrator and Project Coordinator
- **Group B**: Dissemination Coordinator and Data Management Plan manager
- **Group C**: WP leader
- **Group D**: Financial manager
- **WP1**: Partners related to the WP1
- **WP2**: Partners related to the WP2
- **WP3**: Partners related to the WP3
- **WP4**: Partners related to the WP4
- **WP5**: Partners related to the WP5
- **WP6**: Partners related to the WP6
- **WP7**: Partners related to the WP7

- The partners are defined as:
  - POLIMI: members affiliated to POLIMI
  - TUW: members affiliated to TUW
  - KELVION: members affiliated to KELVION
  - EXERGY: members affiliated to EXERGY
  - USE: members affiliated to USE
  - CITY: members affiliated to CITY
  - QUANTIS: members affiliated to QUANTIS
  - ABENGOA: members affiliated to ABENGOA
  - UNIBS: members affiliated to UNIBS

There are two access levels to each folder: Read (**R**) and Write (**W**). Each folder has a defined structure of 'read' and 'write' access levels defined in the access matrix. The access matrix for the first folder structure is displayed below.

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			A		B		C		D		WP1		WP2		WP3		WP4		WP5		WP6		WP7	
			Administrador Leve		Coordinator Level		WP leader Leve		Financial															
	Folder (level 0)	Subfolder (level 1)	R	W	R	W	R	W			R	W	R	W	R	W	R	W	R	W	R	W	R	W
1	General Info		x	x	x	x	x		x		x		x		x		x		x		x		x	
		Contractual documents	x	x	x	x	x		x		x		x		x		x		x		x		x	
		Templates	x	x	x	x	x		x		x		x		x		x		x		x		x	
		Logos	x	x	x	x	x		x		x		x		x		x		x		x		x	
2	Work Package		x	x																				
		01 WP1									x	x												
		02 WP2											x	x										
		03 WP3													x	x								
		04 WP4															x	x						
		05 WP5																	x	x				
		06 WP6																			x	x		
		07 WP7																					x	x
		08 WP8									x	x	x	x	x	x	x	x	x	x	x	x	x	x
3	Deliverables		x	x	x	x	x	x			x	x	x	x	x	x	x	x	x	x	x	x	x	x
4	Financial		x	x	x	x			x	x														
5	Meetings		x	x	x	x	x	x			x	x	x	x	x	x	x	x	x	x	x	x	x	x
		20190410-Brussels																						
6	Images		x	x	x	x	x	x			x	x	x	x	x	x	x	x	x	x	x	x	x	x
		DATE-PLACE																						
7	File-exchange		x	x																				
		Under request																						
8	Publications		x	x	x	x	x	x			x	x	x	x	x	x	x	x	x	x	x	x	x	x

Figure 1 - Access Matrix

6 Data Management

The project coordinator will be responsible for keeping the repository updated except for the subfolders corresponding to each Work Package, which have to be updated by the corresponding WP leader. For the correct work flow of the project, it is mandatory to upload all relevant information, and to keep it up to date.

7 Document coding

To simplify and to unequivocally define a specific document or folder, the SCARABEUS documents uploaded in the Deliverables, Meetings and Image folders have to comply with the guidelines listed below.

Deliverables:
DX.YY-conf-LeadBeneficiary-Title
X: WP number
YY: deliverable number
conf: dissemination level[1]
LeadBeneficiary: Organization responsible of the deliverable

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Title: Title of the deliverable according to the DoA
Example for this document:
D7.02-PU-Abengoa-Preliminary Data Management Plan

Meeting Folder:
Date-Place-Type
Date: YYYYMMDD
YYYY: year
MM: month
DD: day
Type:
KoM: Kick of Meeting
GA: General Assembly
CRM: Contractual Review Meeting
TC: Teleconference
Example for the kick-off meeting held in Brussels on April 10th 2019:
20190410-Brussels-KoM

Meeting documents:
SCARABEUS-##type-CODE-RX.Y_Extra
##: unique number in 2 digits starting from 01
Type: Meeting type
KoM: Kick of Meeting
GA: General Assembly
CRM: Contractual Review Meeting
TC: Teleconference
CODE: code for the type of document
AGD: Agenda
MOM: Minutes of Meeting
WP#: from WP1 to WP8 for WP presentations
RX.Y: Release version number (optional)
X: official version
Y: internal and draft version
Extra: additional, relevant information (optional)
Example for the minutes of meeting of the General Assembly:
SCARABEUS-05GA-MOM-R1.2_AE

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8 OPEN DATA PILOT

The SCARABEUS consortium applied for the Open Data PILOT to share the experimental results obtained in the project along with information about the modelling of power systems using CO_2 blends. This is aimed at enabling replication and verification by other members of the scientific community.

The consortium has already identified gaps in the open literature about CO_2 blends regarding both the availability of experimental results and accurate information about modelling approaches. Therefore, sharing the outcome of SCARABEUS would help bridge this gap, hence allowing researchers to reuse these data for their own objectives. It must be pointed out that the primary purpose of the consortium is to protect the new knowledge (Intellectual Property) produced during the project, while sharing the project results with the scientific and industrial communities.

In this final data management plan, a description of the main data which will be made available is reported together with information about who is responsible for sharing the data.

Chair person

Giampaolo Manzolini be chairing the Open Data PILOT for the consortium, providing indications and suggestions of the type of data to be shared. Also, the Chair Person will create the necessary environment in the selected Open repository to link the uploaded data to the Scarabeus project.

Responsibilities and timing

Each partner will be responsible for the Open data generated within the institution/company and for uploading it to the open repository. The following approach will be adopted throughout the entire project as well as for publications which will occur after the completion of the project:

- When the results are generated, the partners (in particular, the academic partners) will report the data in an open-access publication as much as possible.
- In correspondence to or after paper publication (if successful) the data will be made available to the open repository. .

Open repository

The open repository cannot be integrated in the internal repository of the project mentioned in sections 1 and 2 of this document due to security reasons. Therefore, alternative, well established platforms for knowledge share must be used instead. The following options were evaluated:

- ZENODO
- Mendeley

Both alternatives have their forte and the final selection is decided to be Zenodo after consulting the preferences of the Consortium Partners.

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ZENODO repository

Zenodo is an open source repository launched in 2013, developed under the European OpenAire program and operated by CERN. This repository provides all the necessary tools to comply with FAIR principles. The FAIR principles were defined in *Wilkinson, M. D. et al. The FAIR Guiding Principles for scientific data management and stewardship. Sci. Data 3:160018 doi: 10.1038/sdata.2016.18 (2016)*. The authors intended to provide guidelines for the Findability, Accessibility, Interoperability and Reusability (FAIR) of digital assets, emphasizing the computational relevance of actual developments. In this sense, Zenodo provides an environment that envisage the FAIR principles, providing a structure and encouraging the authors to ensure the FAIRness of the uploaded data.

To be Findable:

- **F1**: (meta)data are assigned a globally unique and persistent identifier
  - A DOI is issued to every published record on Zenodo.
- **F2**: data are described with rich metadata (defined by R1 below)
  - Zenodo's metadata is compliant with DataCite's Metadata Schema minimum and recommended terms, with a few additional enrichements.
- **F3**: metadata clearly and explicitly include the identifier of the data it describes
  - The DOI is a top-level and a mandatory field in the metadata of each record.
- **F4**: (meta)data are registered or indexed in a searchable resource
  - Metadata of each record is indexed and searchable directly in Zenodo's search engine immediately after publishing.
  - Metadata of each record is sent to DataCite servers during DOI registration and indexed there.

To be Accessible:

- **A1**: (meta)data are retrievable by their identifier using a standardized communications protocol
  - Metadata for individual records as well as record collections are harvestable using the OAI-PMH protocol by the record identifier and the collection name.
  - Metadata is also retrievable through the public REST API.
- **A1.1**: the protocol is open, free, and universally implementable
  - See point A1. OAI-PMH and REST are open, free and univesal protocols for information retrieval on the web.
- **A1.2**: the protocol allows for an authentication and authorization procedure, where necessary
  - Metadata are publicly accessible and licensed under public domain. No authorization is ever necessary to retrieve it.
- **A2**: metadata are accessible, even when the data are no longer available
  - Data and metadta will be retained for the lifetime of the repository. This is currently the lifetime of the host laboratory CERN, which currently has an experimental programme defined for the next 20 years at least.
  - Metadata are stored in high-availability database servers at CERN, which are separate to the data itself.

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To be Interoperable:

- **I1**: (meta)data use a formal, accessible, shared, and broadly applicable language for knowledge representation.
  - Zenodo uses JSON Schema as internal representation of metadata and offers export to other popular formats such as Dublin Core or MARCXML.
- **I2**: (meta)data use vocabularies that follow FAIR principles
  - For certain terms we refer to open, external vocabularies, e.g.: license (Open Definition), funders (FundRef) and grants (OpenAIRE).
- **I3**: (meta)data include qualified references to other (meta)data
  - Each referrenced external piece of metadata is qualified by a resolvable URL.

To be Reusable:

- **R1**: (meta)data are richly described with a plurality of accurate and relevant attributes
  - Each record contains a minimum of DataCite's mandatory terms, with optionally additional DataCite recommended terms and Zenodo's enrichments.
- **R1.1**: (meta)data are released with a clear and accessible data usage license
  - License is one of the mandatory terms in Zenodo's metadata, and is referring to an Open Definition license.
  - Data downloaded by the users is subject to the license specified in the metadata by the uploader.
- **R1.2**: (meta)data are associated with detailed provenance
  - All data and metadata uploaded is tracable to a registered Zenodo user.
  - Metadata can optionally describe the original authors of the published work.
- **R1.3**: (meta)data meet domain-relevant community standards
  - Zenodo is not a domain-specific repository, yet through compliance with DataCite's Metadata Schema, metadata meets one of the broadest cross-domain standards available.

Extract form the webpage of Zenodo

The Consortium Partners agree to comply as much as possible with these FAIR principles.

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Project outcome to be included in the Open Data PILOT

The following project results will be included in the Open Data PILOT

Partner	Type of information	Why is it relevant	When
POLIMI	Vapour-Liquid Equilibrium data for CO2 based mixtures (See Appendix 1)	New VLE data for these blends are needed to predict their thermodynamic properties, via calibrated Equations of State, useful for equipment sizing and design	Around M24 for the first fluid candidates, around M36 for other fluid candidates
	Equation of state formulation for the blends	Equations of state validated on experimental results are mandatory to correctly predict the fluid behaviour and the power cycle performance	Around M24 for the first fluid candidates, around M36 for other fluid candidates
TUW	Results of test tube measurements, pure CO2, blend 0	comparison to other experimental research	M40
	Results of whole test rig, blend 1, 2; standard and optimized PCHE	comparison to other experimental research	Within 1 year after the end of the project
	Information about modelling CO2 as a working fluid in Apros simulation software	knowledge of how to use dynamic simulations for similar projects is useful to other researchers	M48
USE	Heat and mass balance of the reference cases for each cycle layout, ambient conditions and mixture composition. Information corresponding to either on design and off-design operation.	With this information, a researcher would be able to validate and benchmark their own performance models and simulations.	On-design, rated performance: M22 Off-design performance: M42
CITY	Information on new turbomachinery design methods for sCO2 turbines (operating with and without blends)	Enhance current design practices and improve understanding to allow sCO2 turbomachinery to be enhanced	Regularly throughout the project

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	Information regarding turbomachinery component cost for sCO2 application		
	Results showing the effect of using sCO2 with blends on the design parameters of the turbomachinery components and their effect on their performance and the overall power plant performance.		
	Improved loss models for turbomachinery components that are operated using CO2		
	Improved correlations for estimating cost of the turbomachinery components for CO2 plants		
QUANTIS	Final LCA results	To share the environmental information related to the CSP technologies	M45
UNIBS	Thermal stability results for CO2 based mixtures (see Appendix 1)	Thermal stability tests identify the maximum operating temperature for these blends, thus the maximum temperature of the power cycle. This information can be used for equipment sizing and design	Around M26 for the first fluid candidates, around M36 for other fluid candidates

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Format of data

The formats adopted for the Open Data will be very different, consistent with the type of data (experiments, modelling) and the corresponding sector. However, for each set of data, a standard exchange format for the sector will be adopted as much as possible. Regardless of the format, the Chair of the Open Data PILOT will make sure that the information provided is complete and enables replication of results.

Conclusions

This document outlines the configuration of a data repository that will be used for the whole duration and after the termination of the project. It is impossible to foresee all the situations that may occur in the future, thus updates to the information in this document will be performed if relevant modifications are implemented.
For the Open Data Pilot, the main characteristics are reported together with the type of information to be included throughout the project. The Zenodo repository is selected to upload all Open Data results.

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Appendix 1: examples of data shared by partners

VLE DATA prepared by POLIMI

The reported quantities are: temperature of the mixture, pressure of the mixture, molar composition of the liquid phase, molar composition of the vapour phase, combined uncertainty on the liquid molar composition, combined uncertainty on the vapour molar composition.

The temperature range of the investigated VLE conditions are from 50°C to 90°C, while the pressure range is from 10 bar to 115 bar.

The VLE molar compositions are investigated through gas chromatography.

Before the measurements, the GC has been calibrated on the molar flow rate of some samples of each one of the pure components.

Point ID	T [K]	P [MPa]	x_{CO2} [-]	y_{CO2} [-]	Ux_{CO2} [-]	Uy_{CO2} [-]
1	363.08	0.9967				
2	363.08	1.5380				
3	363.08	2.0048				
4	363.08	2.5620				
5	363.08	3.0188				
6	363.08	3.5257				
7	363.08	4.0226				
8	363.08	4.5158				
9	363.08	5.0046				
10	363.08	5.5198				
11	363.08	6.0062				
12	363.08	6.5633				
13	363.08	7.0790				
14	363.08	7.5735				
15	363.08	8.0812				
16	363.08	8.6014				
17	363.08	9.0132				
18	363.08	9.5200				
19	363.08	10.0046				
20	363.08	10.5056				
21	363.08	11.0140				
22	363.08	11.4033				
1	343.25	1.0436				
2	343.25	1.5001				
3	343.25	2.0033				
4	343.25	2.5301				
5	343.25	3.0692				
6	343.25	3.5086				
7	343.25	4.0235				
8	343.25	4.5196				
9	343.25	5.0218				
10	343.25	5.5248				
11	343.25	6.0222				
12	343.25	6.6010				
13	343.25	6.9903				
14	343.25	7.5004				
15	343.25	8.0075				
16	343.25	8.6435				
17	343.25	9.0057				
18	343.25	9.4533				
19	343.25	9.9470				
20	343.25	10.4669				
1	323.15	1.0306				
2	323.15	2.0151				
3	323.15	3.0094				
4	323.15	4.0077				
5	323.15	5.0143				
6	323.15	6.0058				
7	323.15	6.9962				
8	323.15	8.0015				
9	323.15	8.5025				

Thermal stability DATA OF CO_2 – X mixture

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In the experimental activity, the measurement starts from the (P,T) condition of the mixtures along an isochoric transformation, before the heating of the fluid (a.k.a. virgin mixture) up to the maximum temperature of interest.

The range of maximum temperature covers 450-650°C, depending on the fluid of interest.

Thermal stability test of the mixture with CO2 blended with C6F6, TiCl4 and C4F10 have been carried out.

Temperature measured	Pressure of the virgin mixture	P of the mixture after 100h at Tmax1	P of the mixture after 100h at Tmax2	P of the mixture after 100h at Tmax3
T1	P1	P1.1	P1.2	P1.3
T2	P2	P2.1	P2.2	P2.3
…	…			
Tn	0Pn	Pn.1	Pn.2	Pn.2

The temperature range where the (P,T) behaviour of the virgin mixtures is tested is around 20°C-200°C.

The results provide the pressures after the cooling of the fluid down to the initial conditions.

The thermal stability is evaluated through a comparison between the pressures of the mixture in virgin conditions and the ones at the same temperatures after the heating phase.

The volume of the mixture is conserved during the whole experimental activity, and therefore the measurements are based on the $P - \rho - T$ behaviour of the mixture: if the $P - \rho - T$ behaviour of the virgin fluid is mimicked after the heating phase, then the mixture can be considered thermally stable up to the maximum investigated temperature Tmax,i.

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