ABraytCSPfuture

Air-Brayton Cycle Concentrated Solar Power future plants via redox oxides-based structured thermochemical heat exchangers / thermal boosters

Deliverable D8.2.
Data Management Plan

Dissemination Level: Public

WP8 Knowledge and innovation management, dissemination, communication and European innovation base development

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https://www.abraytcspfuture.eu/

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Disclaimer

The work described in this document has been conducted within the ABraytCSPfuture project that is co-funded by the European Union. Views and opinions expressed herein are however those of the author(s) only and do not necessarily reflect those of the European Union or of the granting authority, European Climate, Infrastructure and Environment Executive Agency (CINEA). Neither the European Union nor the granting authority can be held responsible for them.

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1.1	28.04.2023	Updated with final partner feedback	Christos Agrafiotis	DLR
1.2	30.04.2023	Final Review	Javier Baigorri Martinez	CENER

About the Project

ABraytCSPfuture sets forth an innovative, carbon-neutral way for implementing the highly efficient air-Brayton gas turbine power generation cycles into future air-operated Concentrated Solar Power (CSP) plants. Air-Brayton cycles are used in traditional power plants where, however, involve fossil fuels combustion via pressurized air. *ABraytCSPfuture*'s carbon-neutral approach aims at achieving higher solar-to-electricity efficiencies, vital for competitiveness of CSP and non-reachable by either PVs or molten salts and thermal oils, increasing in parallel significantly the plants' storage capability. The project will develop and demonstrate a first-of-its-kind compact, dual-bed thermochemical reactor/heat exchanger unit that will transfer heat from a non-pressurised air stream to a pressurised one, while also operating as a thermal booster, raising the temperature of the pressurized stream to the level required for Brayton cycles. Furthermore, the volumetric solar energy storage density of air-operated CSP plants will be significantly increased by rendering their current sensible-only regenerative storage systems to hybrid sensible-thermochemical storage ones within the same storage volume. Both these functionalities will be materialized by thermochemical reactor/heat exchanger units comprised of non-moving, flow-through porous ceramic structures (honeycombs or foams) based on earth-abundant, cost-efficient, non-toxic oxide materials and exploiting reversible reduction/oxidation reactions of such oxides in direct contact with air, accompanied by significant endothermic/exothermic heat effects. The proposed technology is set forth by an interdisciplinary partnership spanning the entire CSP value chain, comprised of leading research centres, universities, innovative SMEs and large enterprises, including ancillary services providers and technology end-users.

Deutsches Zentrum fuer Luft- und Raumfahrt e.V., **DLR**	DE	
Centre for Research & Technology Hellas, **CERTH**	EL	
University of Twente, **UT**	NL	
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COBRA Instalaciones y Servicios S.A., **COBRA**	ES	

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This deliverable is part of a project that has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement no 1010845.

Executive Summary

The present document constitutes the first version of Deliverable D8.2 "*Data Management Plan*" developed within WP8 of the HORIZON EUROPE 2020 ABraytCSPfuture project. It describes the creation of the Data Management Plan (DMP) for the data to be generated and used in the context of the project. This version of DMP, created early in the project, will serve as a basis to define the processes followed by each partner with respect to data management as well as to draft the data management strategy at project level. It is going to be revised twice (as part of the interim and final project review) and fine-tuned to the data generated then and the uses identified by the consortium.

As part of making research data FAIR compliant (i.e. findable, accessible, interoperable and re-usable), D8.2 includes information and clear descriptions about:

(a) the kind of data sets that will be generated, collected and processed;

(b) the main criteria set to distinguish among the data as (1) private, (2) publishable and (3) Open Access;

(c) the adopted methodologies and standards to be applied;

(d) the consortium's policy on data sharing;

(e) processes of data handling/archiving/preservation during/beyond the project and metadata produced, to manage the lifecycle of datasets collected.

Changes with respect to the DoA

No changes or Deviations from the Work plan occurred with respect to this Deliverable *D8.2 Data Management Plan*.

1. Introduction

Deliverable D8.2 "*Data Management Plan*" is produced within *WP8 Knowledge and innovation management, dissemination, communication and European innovation base development,* of the ABraytCSPfuture project, with the purpose of outlining the approach to be adopted during and after the project for relevant data acquisition, organisation and sharing. The document is based on the Description of Work (DoW) in the proposal and its modifications during the Grant Agreement preparation procedure and is drafted based on the template provided by Horizon Europe online manual. In this context, the specific objectives of this deliverable are:

- To identify the datasets that the project will generate through its course and group them in a rational manner.
- To establish the processes for ensuring that the data will be made 'FAIR' (Findable, Accessible, Interoperable and Reusable).
- To ensure solid data management according to the FAIR principles and the General Data Protection Regulation (GDPR).
- To define procedures for data handling/archiving/preservation during and beyond the project.
- To draft and further elaborate the Consortium's policy for data sharing.

The DMP will evolve during the lifetime of the project to include renewed insights in the data management.

2. Data Summary

Types, formats and origin of data that the project will generate/collect: Both experimental as well as numerical research data will be generated from the partners themselves during the project, from:

- the lab tests and characterisations,
- the synthesis of oxide multi-component powders and their shaping to porous structured objects,
- the modelling, operation simulation and relevant proof-of-concept demonstration campaigns of thermochemical management of redox chemical reactions,
- the TEA/LCA tasks.

Such data will include among others, redox oxide materials computational screening and synthesis/shaping protocols, thermophysical/thermomechanical properties, kinetics/ thermodynamics data, process simulation and automation outputs and LCA data.

The origin of the data depends on the specific dataset. Table 1 contains an indicative initial list of types of datasets expected to be generated and managed along the evolution of the ABraytCSPfuture project, together with their origin and the partners foreseen to generate them.

Table 1: First classification and indicative examples of types of datasets to be created and managed within the ABraytCSPfuture project from project partners.

No	Dataset/research output	Data type	Origin of data	Partners involved
1	Atomistic scale simulations files	*.cif; *.pw.x; *.json	Use of special open source and licensed "data mining" platforms.	DLR, CERTH, FHG
2	Computer codes (materials screening)	MATLAB, Python scripts (*.py)	Use of existing open source databases and new, in-house generated python scripts.	DLR, CERTH, FHG
3	Materials Structural analysis with FEM	ANSYS, OPENFOAM	Use of open source and licensed software.	DLR, TEKN
4	Material characterisation files (e.g. SEM pictures, crystallographic data etc.) generated by various analytical instruments	*.png, *.jpg, *.tiff, ASCII, *.csv, *.opg, etc.	Use of relevant characterisation and analytical instruments.	DLR, CERTH, FHG
5	Synthesis recipes and shaping protocols	*.txt, *.doc, etc.	Experiments performed and relevant laboratory records.	DLR, CERTH,
6	CAD files of reactor/test rigs designed, blueprint files	Autodesk Inventor (*.ipt, *.iam, *.idw), *.stp, *.iges, etc.	Use of open source and licensed software.	DLR, CERTH, KB, LET
7	Graphics files	Visio, Draw.io etc.	Use of open source and licensed software.	All partners
8	CFD analysis files	OPENFOAM, ANSYS (FLUENT)	Use of open source and licensed software.	DLR, UT, TEKN

9	Piping and Instrumentation diagrams (P&ID) files	SmartDraw e.g. *.edraw	Use of open source and licensed software.	DLR, CERTH, KB,
10	Process simulation files	ASPEN, COMSOL, DYMOLA	Use of open source and licensed software.	DLR, CERTH, UT, CENER, TEKN,
11	Automation files (data logging and control software)	Labview virtual instrument files (*.vi)	Use of open source and licensed software.	DLR, CERTH, CENER, TEKN,
12	TEA/LCA data files	OpenLCA, GaBi, Umberto files, Excel	Existing literature and partners own analysis using open source and licensed software.	DLR, FHG
13	Stakeholders database	Excel, Word	Partners input.	FHG
14	Reports, documents	Word, Excel, Power point, PDF	Partners input.	All partners
15	Statistical data from dissemination activities	Word, Excel	Partners input.	DLR, CENER

Purpose of the data collection/generation and its relation to the objectives of the project: All these groups of data to be collected are necessary and will be used for the successful implementation of the various research tasks of the project. Specifically:

- The atomistic-scale simulations results will be employed for computational "materials-by-design" screening and selection of material compositions to guide the experimental synthesis tasks avoiding costly and lengthy experiments.
- The structural analysis data, for the prediction of thermochemical stresses and the consequent optimal design of the porous structures to be produced, in order to be able to tolerate and accommodate them.
- The material characterisation data in order to understand and fine -tune the properties of the oxides synthesized and their variation with operating conditions, as well as for comparison to theoretical/modeling predictions.
- The synthesis recipes and shaping protocols to establish reliable, reproducible, scalable and environmental-friendly synthesis and shaping routes.
- The CAD, graphics, P&ID and automation data will be used for the design and operation of the core project's Deliverable, the dual-bed pressurized unit.
- The process simulation data, for comparison with experimental ones and validation of the simulation models in a feedback process.

- The LCA data, to guideline the materials selection providing relevant eco-friendly and cost-effective solutions roadmaps and the TEA ones in an overall performance assessment of the technology of such future air-operated STPPs vs. other "state-of-the-art" fluid-based systems in terms of cost, efficiency, maintenance etc.
- The stakeholders' database for the purposes of assessing the environmental, social and economic impact of the project's results and appraise policy options for accelerating diffusion of the technology through a wider stakeholder/public engagement.

All data above will also be used for the "transversal" project activities, i.e.:

- Communication and dissemination of the project results.
- Articulation of the exploitation strategy for key exploitable project results.
- Management of IPR inside the consortium.
- Overall project management.

Expected size of the data: Overall, the project is expected to generate < 1 TB of data. Naturally at this stage, this figure is a rough estimate and a more accurate number will be available upon the project's progress.

Re-use of any existing data: In the course of the project and depending on its needs, pre-existing open research data/software/algorithms might be used, like, e.g. available online "data mining" databases like Materials Project (www.materialsproject.org) into which DLR has already introduced relevant data. Additionally, TEA and LCA activities, will reuse previous data, methodologies or templates spanning the main research areas addressed in the project, e.g. raw materials, CSP and RE in general, to facilitate the relevant work.

'Data utility': Obviously, the data generated will be directly useful for the consortium partners, guiding their activities towards the achievement of the project's technical goals. Furthermore, on the one hand, the "sensitive" ones will be employed to identify Key Exploitable Results of the project and establishing relevant IPR strategies. On the other hand, the data eventually published in the form of articles in scientific journals and conference presentations will be useful for the research and industrial community active in the fields addressed within the project, i.e. materials science and engineering, oxide ceramics synthesis and shaping, design and implementation of thermochemical engineering processes, and CSP and RE in general to name a few. Overall, the generated data will be useful to the first list of main potential stakeholders and industrial end users identified in the "Impact" section of the Project, namely:

- Shaped ceramics industry.
- Gas turbine developers.
- CSP/PV plant development companies and EPC contractors of key components in power plants.
- Industrial processes with high temperature waste heat (cement, steel, glass).
- Grid and Transmission System Operators (TSOs).
- Political/ governmental authorities.
- Public communities.

3. FAIR data

3.1 Making data findable, including provisions for metadata

Provisions and actions that will be taken to ensure the discoverability of ABraytCSPfuture data include accompanying datasets with properly structured and accurate metadata according to FAIR data principles and/or making them identifiable by using standard identification mechanisms where applicable. For the latter case, persistent identifiers (either Digital Object Identifiers/DOIs, or Uniform Resource Names/URNs) provided by the data repository will be used as well as ORCID researchers' identifiers. Several datasets will be linked to respective Digital Object Identifiers (DOIs). Those for the scientific publications for example, will be provided from the publisher, while for other literature (e.g. reports etc.) will be assigned via the repository in which they will be archived. Published and FAIR-compliant data will be archived in open data trusted repository options, such as Zenodo, a joint collaborative effort of CERN, the OpenAIRE initiative and the European Commission (https://zenodo.org/). Therein, all uploads/ published data sets are associated with standard Zenodo metadata, which are by default:

- Digital Object Identifiers.
- Version numbers.
- Bibliographic information.
- Keywords.
- Abstract/description.
- Associated project and community.
- Associated publications and reports and their types (e.g. Publication, Poster, Presentation, Dataset, Video/Audio etc.) with mandatory basic information: publication date, title, authors, description (abstract).
- Funding: Grant programme name and number.
- Access and licensing info: access rights (open, embargoed, restricted, closed access), license name (Creative Commons versions).
- Language.

In addition, links for all project's uploads to the Open Access Research Data repository initiated by the European Commission (Open AIRE https://www.openaire.eu/) is envisaged. Each partner will be responsible for uploading public datasets that they have generated and assign specific keywords relevant to these datasets.

3.2 Making data openly accessible

The project partners will take all efforts to make as much as possible project-generated data openly available and usable for third parties for study, teaching and research purposes. All reports and data associated with the project's Public (PU) Deliverables, that are not confidential will be made in principle available. Exceptions and possible embargo time, relevant to potential of scientific publications, the protection of

partners' IPR and potential commercial exploitation will be decided by the consortium as foreseen in the respective Grant Agreement and Consortium Agreement. Other exceptions are associated with the findings of three non-public, Sensitive (SEN) Deliverables identified as relevant for potential exploitation from the partners, stated explicitly in Table 2 below.

Table 2: Sensitive, non-public Deliverables and respective reason.

Deliverable	Deliverable name	Reasons for exception
D2.4	Optimized redox oxide powder formulations for model ceramic pieces manufacture.	• Potential patenting the stoichiometry of optimized "recipes" to improve thermal expansion/ contraction properties of perovskite compositions.
D3.2	Optimal porous structures for combined TCS/thermal booster operation based on combined activity, thermo-mechanical stability and cyclability performance.	• Potential patenting of production method(s) of perovskites porous structured objects with high oxide content and of recycled oxides from the partners involved. • Licencing to major ceramic companies.
D3.3	Optimized redox oxide formulations and structured objects for proof-of-concept-scale unit.	• Developing a platform of redox perovskite compositions for industrial users for a variety of applications: TCS, chemical looping concepts, catalysis etc.

Furthermore, additional datasets from those included in Table 1, can be during their generation judged as of potentially having commercial value for the partner(s) generating them and thus worthy of further protection methods. Indicative, but not exhaustive examples include CAD and structural analysis files for the design of the thermochemical reactors and process simulation files related to them.

As already mentioned, in order to render project results and associated metadata easily findable and accessible, it is envisaged that data will be archived in the Zenodo open data trusted repository. This platform is very commonly used for sharing research results from EC-funded projects following the FAIR principles. Publications or other research results, can be added therein under open, closed, or embargoed access, enabling sharing of the latter not immediately, but only after a certain time.

In addition to Zenodo, some partners may make use of their own research publication open repositories. For example, DLR supports the Open Access principle with the introduction of its own open current research information system ELIB (Electronic Library System) https://elib.dlr.de/ where self-archiving of all publications of its

personnel is mandatory (sometimes after a short embargo period, depending on the publisher's contract) – in full accordance with the Green Open Access model; these publications are publicly available and accessible through external searches.

3.3 Making data interoperable

Interoperability of generated data will be ensured by following metadata vocabularies, standards, formats and methodologies commonly endorsed or considered as standard from those using these data, and by depositing them in a repository that uses the same data and metadata vocabularies. As already stated, the most probable solution is to use the Zenodo repository, which offers export of its internal representation of metadata to other popular formats. In cases where it is unavoidable to use uncommon ontologies or generate project-specific ones these will be openly published alongside the open datasets.

3.4 Increase data re-use (through clarifying licenses)

All reports and data that are not confidential will be licensed under the Creative Commons licenses CC-BY-SA or CC-BY that are used for open publications and relevant open datasets, secure re-use of data/research outputs and also include relevant disclaimers of liability for such re-use. The project partners will provide the relevant documentation needed to validate the data analysis and facilitate data re-use, basically in the relevant publications and as part of the publicly available datasets in the Zenodo repository. Obviously, upon their availability as Open Access in these sources, data can be used by third parties, even after the end of the project. Again, as elaborated above, in case it is envisaged that scientific publications will be produced from certain data, then an embargo period will be applied until these are accepted by the publisher, that will concern also the relevant documentation for the data analysis and re-use. Analogous restrictions with respect to immediate public availability will apply to the data identified as of potential commercial value mentioned in Section 3.2.

4. Allocation of resources

The Gold Open Access model is foreseen to be used widely from the project partners when submitting manuscripts to journals. The relevant fees foreseen from several publishing houses (2,000-3000 €/paper published) have been included in the budgets of all research institutes and university partners of the consortium (2-3 such publications per partner). For the three partners in Germany (including the coordinator), fees for Open Access publications with major academic publishers Wiley and Springer are already covered through a nationwide agreement (DEAL). Alternatively, publications in Open Access Journals free of costs will also be explored. Industrial partners of the consortium

may use part of their project budget to file any necessary patents for protecting their intellectual property.

The Zenodo open data trusted repository envisaged for archiving the date generated, is free of charge. Furthermore, the teamsite created by the Project Coordinator, DLR in its own intranet domain for efficient communication and exchange of information among the partners, is meant to function also as a data repository. All partners have been granted password-protected access to it and capability of uploading/downloading documents that can be stored and exchanged therein. Being part of the coordinator's internal project management system, this "teamsite-repository" does not induce any extra costs to the project or the partners.

Each partner will appoint a person of its research team involved in the project, as responsible for data management and data assurance for their organization.

The resources and terms for long-term preservation of the data will be discussed among the consortium partners at a later stage of the project. Such issues will involve, for example, the maintenance of the Project's website (including the public deliverables) and social media accounts and the sharing of data deposited after the official end date of the project. The outcomes of these discussions will be included in the following, updated versions of the DMP.

5. Data security

During the project, consortium partners will be responsible for managing datasets securely at their possession. Each partner possesses its own security system, but in general, rely on local, protected servers with additional back-up service.

The data available at the project's public website https://www.abraytcspfuture.eu/ created and maintained by CENER and those in the teamsite created and maintained by DLR, are subjected to the data security, backup and recovery mechanisms of the respective hosts.

With respect to long-term preservation and curation spanning after the project's end, as already mentioned it is currently envisaged that data will be archived in the Zenodo open data trusted repository. This repository wherein data and metadata of the project will be retained, is created and maintained by CERN, in Switzerland and consequently its lifetime is that of the host laboratory, i.e. spans at least the next 20 years.

6. Ethical aspects

There are currently no ethical aspects identified within the ABraytCSPfuture project. Even though currently no questionnaires to be distributed to stakeholders are foreseen, in the case that such an activity will be judged as necessary to take place eventually and

the relevant data are agreed to be made public, suitable anonymisation techniques will be applied prior to data archiving.

All project-related dissemination activities involving distribution of project material/information to third parties will be designed to ensure a priori compliance to the elements/requirements of the EU General Data Protection Regulation (GDPR).

7. Other issues

No other issues identified.

8. Conclusions

The present Deliverable comprises the first version of the Data Management Plan (DMP) for the ABraytCSPfuture project, envisaged to evolve during the lifetime of the project in order to include renewed insights in the data management.

At first, the datasets that the project will generate through its course are identified and grouped following the evolution of the project. Then, the processes to be followed for rendering these data FAIR' (Findable, Accessible, Interoperable and Reusable) are established and procedures for data handling/archiving/preservation during and beyond the project are discussed.

All research and academic partners are strongly committed to promote open science policies, principles and research practices, encouraging their researchers to publish results and interpretations of their research in an open and transparent manner, yet respecting on the other hand confidentiality when this is required due to legitimate obligations (for example, with respect to the findings of three non-public deliverables identified as relevant for potential exploitation from the partners). In parallel, the consortium has appropriate technical and organizational skills and measures in place for data protection during the project. All partners are also committed to provide relevant metadata and their documentation to facilitate data's re-use and interoperability.