MOJITO - DECARBONIZED LIME PRODUCTION THROUGH ENHANCED JOINT DIELECTRIC HEATING AND WASTE CARBONACEOUS MATERIAL ADDITION

HORIZON-EIC-2024-PATHFINDERCHALLENGES-01-02 - GRANT AGREEMENT NUMBER: 101221957

Deliverable D1.2:

Data Management Plan

Dissemination Level		
PU	Public	*x*
SEN	Sensitive, limited under the conditions of the Grant Agreement	

Document Type		
R	Document, report (excluding the periodic and final reports)	*x*
DEM	Demonstrator, pilot, prototype, plan designs	
DEC	Websites, patents filing, press & media actions, videos, etc.	
DATA	Data sets, microdata, etc.	
DMP	Data management plan	*x*
ETHICS	Deliverables related to ethics issues.	
SECURITY	Deliverables related to security issues	
OTHER	Software, technical diagram, algorithms, models, etc.	

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General Information

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Project Duration: 3 years
Project website: https://www.mojito-project.eu/

MOJITO consortium

Short	Beneficiary	Role
UNIBO	Alma Mater Studiorum – Università di Bologna	CO
FRA	Fraunhofer UMSICHT	BEN

CO…Coordinator, BEN…Beneficiary, AP…Associated Partner

FOR INTERNAL DOCUMENTATION PURPOSES					
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2	29/03/2026	Version 2.0	24	X	X

Scheduled Data Management Plan (DMP) Updates

The DMP is a document that evolves during the lifespan of the project and registers all relevant changes in the life-cycle of all the research datasets. Updated versions of the DMP have already been planned (see table below). Moreover, this document will be updated whenever important changes in the data or the data management policy occur.

Issue	Expected by project month (M)
Initial DMP (deliverable D1.2)	M6
Intermediate DMP (internal only)	M24
Final DMP (deliverable D1.8)	M36

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Executive Summary

This Data Management Plan (DMP) is a document that provides details on all the research data collected and generated within the MOJITO project. In particular, it explains the way research data are handled, organized, licensed and made available to the public, and how they will be preserved after the project is completed. The DMP also provides motivations when versions or parts of the project research data cannot be openly shared.
This DMP reflects the current state of the art of the MOJITO project. However, the details and the final number of datasets may vary during the research project. The variations will be recorded in updated versions of this DMP.

1 Data Summary

The MOJITO project aims to validate a laboratory scale system to produce decarbonized lime with reduced energy consumption and carbon emissions in the calcination process, while achieving CO_2 removal. The system is based on an electrically powered rotary kiln that transfers heat to the calcining material by microwave and electrical heating. The input material will be integrated with carbonaceous material for its ability to absorb electromagnetic energy and convert it to heat, thus improving the efficiency of the process. Accurate atomistic computer simulations of the $CaCO_3$ calcination process in realistic conditions through machine learning will be performed using a Tier-0 supercomputer. The project will study a first-of-the-kind process, so no previous data exists.
The project will produce different types of data by using different methodologies:

1. Experimental and observational data (numerical, quantitative). Data from laboratory and process measurements.
2. Computational data (textual). Ab initio computational data to study the MOJITO process at the atomistic level.
3. Graphical data (drawings, pictures). Data from prototype design. Data from COMSOL simulation.
4. Textual documents.

Research teams have agreed to convert research data from proprietary formats to well-known and documented open formats in order to facilitate accessibility and reusability (see Table 1).

Table 1. Summary of data formats.

Type of data	**Formats used during data processing**	**Formats for sharing, reuse and preservation**
Experimental and observational data	Proprietary (e.g., Excel .xlsx/.xlsm; NOMAD)	Databases in open formats (e.g., MySQL, .csv)
Computational data	Proprietary	Plain-text
Graphical data	Proprietary (e.g. Illustrator, AutoCAD, COMSOL)	Graphics in open formats (.pdf)
Textual documents	MSWord, .odt, .rtf, .pdf	Open (LibreOffice), .pdf

README files[1] explaining all relevant details regarding data collection, processing methodologies and quality assurance will be deposited, if needed, along with the datasets in .odt, .rtf or .pdf format.
The expected size of the data is about 40 Gigabytes (GB). Considering the early stage of the project, the effective size may vary with respect to what is declared here. Potential variations will be addressed in further versions of this document.
The data produced can be of interest to different potential users. They may include companies producing lime and cement, cement composition, biochar and/or fossil waste, construction and architecture, microwave (MW) technologies, CO_2 management.

2 FAIR Data

This DMP follows EU guidelines[2] and describes data management procedures according to FAIR principles[3]. The acronym FAIR stands for "findable, accessible, interoperable and re-useable", and describe data management practices that allow maximum knowledge circulation and return on investment.

2.1 Making data findable

To improve the findability of research data produced during the project, numerical datasets will be deposited in a trusted data repository, namely NOMAD[4], if and when appropriate. In addition, whenever project results are published, the team members deposit and describe the relative underlying datasets in trusted data repositories in order to guarantee their discoverability, access and preservation beyond the project end. Pure text documents (deliverables, papers) will be deposited in Zenodo (https://zenodo.org).
The chosen repositories (see section 2.2, Table 2) attribute a unique persistent identifier (PID) to the deposited items. The unique identifiers are then used to cite the datasets within all research publications.
They also support standard descriptive metadata to ensure datasets indexing and discoverability. As an example, metadata will be present as encoded in NOMAD Metainfo, which contains also specific schemes for computational data[5].
Specific keywords will be associated to each dataset to enhance semantic discoverability. Thesauri and controlled vocabularies, specifically adapted to environmental data (e.g., https://www.usgs.gov/data-management/keywords) will be used.
Research data are organized in datasets, which are named collections of data units with the same focus and scope. In this DMP we set out common rules for dataset naming, in order to improve data visibility, discoverability, citation and permanent online tracking.
The recommended dataset title structure consists of:
MOJITO_WPn_Tn.n_[brief description]_ver

[1] A "README" file is a document containing relevant information about dataset authorship, terms of reuse and responsibilities, explaining dataset content and structure, collection procedures and analysis (such as file specifics, methodologies, codebooks of variables, data sources, and further necessary notes). (See Annex II to visualize the suggested README file template).
[2] Horizon Europe Programme Guide: https://ec.europa.eu/info/funding-tenders/opportunities/docs/2021-2027/horizon/guidance/programme-guide_horizon_en.pdf
[3] The FAIR data principles (GOFAIR), https://www.go-fair.org/fair-principles/
[4] https://nomad-lab.eu/prod/v1/docs/tutorial/ NOMAD_ELN.html
[5] https://nomad-lab.eu/prod/v1/docs/examples/computational_data/metainfo.html

The version number of the dataset will be added at the end of the title in case of data revisions to help identifying the dataset updates especially in repositories that do not track versioning automatically (see Annex I).
This DMP also recommends the following rules for file naming:

- for dataset file(s): MOJITO_WPn_Tn.n_*[brief description]_ Date(YYYYMMDD)_vers.ext*
- for README file(s)*:* MOJITO_WPn_Tn.n_*[brief description]_Date(YYYYMMDD)_vers_README.ext*

2.2 Making data accessible

As a guiding principle, MOJITO seeks to make all research data openly available as soon as possible and ensure open access — via the repository — in order to allow dissemination, validation and re-use of research results.
To this purpose, all possible and legitimate actions and strategies are adopted to allow data sharing including:

- converting the files to standard open formats;
- providing all relevant documentation and explanation for the data and the datasets;
- obtaining copyright permissions from third party data owners to be allowed to re-use, reproduce and distribute the collected data;
- anonymizing and aggregating the data;
- in case of copyright on raw data derived, collected or elaborated from pre-existing databases or from other original sources (i.e. papers, journal articles, book chapters, reports, video and audio sources), collected data will be made available if the reproduction and sharing are allowed by expressed permission of the right holders or by applicable copyright exceptions and exemptions. Otherwise, only aggregate data resulting from the analysis will be openly published. When the sources are freely available on-line in their original repositories, but direct reproduction is not allowed, a detailed account on how the dataset was created from the original data will be provided, together with the specification of open repositories from where the original datasets are available. Raw data consisting in full texts will not be made available without the copyright holders' permission.

Restrictions to access are applied only in the following cases:

- collected data belong to third party which have denied permission for sharing on account of confidentiality and proprietary issues;
- data anonymization is not possible;
- data availability would jeopardize the project's main aim.

See Annex I for details on the accessibility of each dataset. In all cases, metadata will be made openly available and licensed under a "No Rights Reserved" CC0 license or equivalent, as per the Grant Agreement, and will contain information on how to access the data.
The data repositories chosen guarantee long term preservation and attribute persistent unique identifiers to the archived datasets. It supports open licenses and different access levels. Finally, it adopts descriptive metadata standards such as Dublin Core and DataCite Metadata Schema, as required by the OpenAIRE guidelines[6], and allow cross-linking between publications and the relevant datasets. Please see Table 2 for more detail on the identified repository.

[6] OpenAIRE, https://guidelines.openaire.eu/en/latest/

Table 2. Summary of repositories.

Partner	Repository name	Type	URL	PID	OpenAIRE compatibility?
UNIBO, Fraunhofer	NOMAD	Disciplinary	https://nomad-lab.eu	DOI	Not yet registered
UNIBO, Fraunhofer	ZENODO	Generalist	https://zenodo.org	DOI	Not yet registered

2.3 Making data interoperable

All datasets will be described using standard descriptive metadata, to ensure metadata interoperability for indexing and discoverability. For each deposited dataset, relevant documentation explaining data collection procedures and analysis is made available along with the data, to guarantee intelligibility, reproducibility and the validation of the project findings.
As mentioned, the team will convert all shareable data from proprietary formats to well-known and documented open formats (see section 1, Table 1). In particular, some of the data will be stored in NOMAD, to profit of the strong disciplinary interoperability of NOMAD Metainfo. Using this repository promotes interoperability and data reuse, also thanks to AI tools, allowing data exchange and re-use between different researchers, institutions, organizations and countries.
No output has been produced yet. Any publication based on the data will be mentioned in later versions of this DMP and will contain a data availability statement.
If specific software is used during data processing, full explanation and instructions will be included in the deposited documentation. As an example, for atomistic data (WP4), the provided input files will allow anyone to re-calculate the data by means of the open-source programs used to generate the data. The details of the adopted methodology, data analysis will be described in the deliverable report and published papers.
See Table 3 for a summary of the tools and software necessary to reuse our data.

Table 3. Summary of tools and software for enabling re-use of the datasets.

Tools/software
Open spreadsheet and document editors, such as OpenOffice[7] or LibreOffice[8]
Free CSV file viewers, such as CSV viewer[9]
Open-source programs

2.4 Increasing data re-use

In general, MOJITO will license data under CC-BY. However, MOJITO will apply the principle 'as open as possible, as closed as necessary', if there are intellectual property rights on data, as well as sensitive or classified data which must be kept close (e.g., through access control mechanisms).
It is possible that an embargo period may be applied to some datasets to allow full exploitation of research results by the team. Any embargoes applied to the datasets are specified in Annex I.

[7] OpenOffice: http://www.openoffice.org/
[8] LibreOffice: https://www.libreoffice.org/
[9] https://csviewer.com/

As per the Grant Agreement, metadata will be openly available under a Creative Commons "No Rights Reserved" (CC0) license or equivalent.
The quality of the data will be carefully assured using different approaches. In particular, double check by two independent analysis teams will be applied as much as possible.

3 Other research outputs

No other output of our research, different from data and publications, is foreseen.

4 Allocation of resources

Making data FAIR requires an investment of money and researchers' time. At this time, the estimated cost, above standard planned research procedures and practices, of processing, storage and sharing data is about 3 to 4 Person-Month (PMs). Long-term preservation cost could be minimal, given the chosen repositories.
Responsibility for data management usually sits with each dataset creator (see Table 4). Table 5 identifies all contributors participating in data management activities and specifies their roles.

Table 4. Summary and contacts of people responsible for data management. (UNIBO-CMU: UNIBO Computational Modelling Unit; UNIBO-TPU: UNIBO-Thermal Processing Unit).

Team	Name	ORCID (if available)	E-mail address
UNIBO-TPU	Marco Melandri		marco.melandri9@unibo.it
UNIBO-CMU	Maria Clelia Righi	0000-0001-5115- 5801	clelia.righi@unibo.it
FRA	Martin Meiller		martin.meiller@umsicht.fraunhofer.de

Table 5. Summary of team members involved in the datasets collection and management.

Team	Name	ORCID (if available)	Role
UNIBO-TPU	Antonio Primante		Team member
UNIBO-TPU	Alessia Alcantarini	0000-0002-9933- 7812	Team member
UNIBO-TPU	Lucio Quadrani	0000-0003-4830-0259	Contributor
...			

See Annex I for details about data management responsibilities related to each dataset.

5 Data security

During active data management (e.g., during data collection and analysis), research data stored in computers, laptops, intranets or hard-drives are accessible only after logging in with username and password (periodically modified according to national law provisions for data security) and are protected by updated antiviruses. They are also regularly backed-up in order avoid accidental losses. None of the project data will ever be left inadvertently available. If external devices are used to store data files (e.g., backup files), they will be kept in a safe place accessible only to the researchers involved or will be encrypted with ad-hoc software.
The cloud storage solution (UNIBO Microsoft SharePoint) will be adopted for data sharing among team members. In this case, too, regular backup of the data will be performed to ensure data recovery.
Long term preservation of public data is ensured by the chosen data repositories that have specific preservation policies.

6 Ethical or legal aspects

There are no envisageable ethical aspects in the data produced by MOJITO. No personal data is included and data are produced expressly for the project, so no copyrighted materials are used.

7 Other issues

No particular issue is foreseen at present.

Annex I: Datasets

The analytic description of each expected dataset of the MOJITO project is included in this Annex.

Dataset ID	MOJITO_WP2_T2.2_carbonate_material_1.0
Task title	Task 2.2 Chemical and physical analysis of input materials
Dataset name	Chemical and physical analysis of carbonate materials
Ready at month of project	M12
Status	In progress
Chosen Repository	NOMAD
PID [PID type]	DOI
Version	1
Task & data manager	UNIBO
Name of other partners involved	FASSA BORTOLO
Creator/s	Melandri Marco [UNIBO-TPU]
Contributor/s	Antonio Primante [UNIBO-TPU], Alessia Alcantarini [UNIBO-TPU], Lucio Quadrani [UNIBO-TPU]
Contact Person/s	Melandri Marco [UNIBO-TPU, marco.melandri9@unibo.it]
Dataset description	This data set contains data with feedstock analysis results from carbonate materials conducted ensuring compliance with the certified standard UNI EN 459-2:2021. FASSA BORTOLO company will provide for the industrial-grade carbonatic material. This analysis evaluates the properties and performance of each input carbonate material, providing essential data to support research and development efforts and enhance product formulation strategies. The analysis results include the concentrations of Na, K, Mg, Ca, Al, Si, P, Fe and heavy metals such as Pb, As, and Cd determined with ICP-OES. Also, analysis results from TGA and elemental analysis carried out using CHNS. Surface area is determined with physisorption and dielectric loss (") along with permittivity (') measured using a dielectric probe. Data from XRD analysis. Data from particle size, bulk density, free water, LOI 1050 and %CaO and %MgO are also provided by FASSA BORTOLO for the delivered material.
Data format	N/A
Data volume	N/A
Data handling standards	Data collection, aggregation, storage and sharing in compliance with Horizon Europe Requirements (FAIR principles)
Metadata	Key words: CaO, MgO, CaCO3, carbonate, ICP-OES, TGA, CHNS, XRD, UNI EN 459-2:2021, surface area, dielectric analysis.
Tools for reuse	N/A
Data security	The data generated are stored with online and offline backups.
Data management cost	¼ PM
Accessibility & data sharing	Public
Copyright & IP management	None
Ethical issues management	In compliance with EU Regulation 2016/679 GDPR
Additional data management procedures	N/A
Related publication/s	None

Dataset ID	MOJITO_WP2_T2.2_carbonaceous_material_1.0
Task title	Task 2.2 Chemical and physical analysis of input materials
Dataset name	Chemical and physical analysis of carbonaceous materials
Ready at month of project	M12
Status	In progress
Chosen Repository	NOMAD
PID [PID type]	DOI
Version	1
Task & data manager	UNIBO
Name of other partners involved	None
Creator/s	Melandri Marco [UNIBO-TPU]
Contributor/s	Antonio Primante [UNIBO-TPU], Alessia Alcantarini [UNIBO-TPU], Lucio Quadrani [UNIBO-TPU]
Contact Person/s	Melandri Marco [UNIBO-TPU, marco.melandri9@unibo.it]
Dataset description	This data set contains data with feedstock analysis results from carbonaceous materials. This analysis evaluates the properties and performance of each input material, providing essential data to support research and development efforts and enhance product formulation strategies. The analysis results of concentrations of Na, K, Mg, Ca, Al, Si, P, Fe according to ISO 23380 and heavy metals such as Pb, As, and Cd according to EN ISO 12846, determined with ICP-OES. Analysis results from TGA and elemental analysis carried out using CHN according to ISO 29541. Sulphur content according to ISO 19579, and Oxygen content according to ISO 17247. Surface area determined with physisorption using ISO 9277/2022. Ash content (550 °C) determined by ISO 1171, DIN 51719: Volatile matter according to ISO 562, DIN 51720. Particle size distribution with ISO 1953 Dielectric loss (”) along with permittivity (’) measured using a dielectric probe.
Data format	N/A
Data volume	N/A
Data handling standards	Data collection, aggregation, storage and sharing in compliance with Horizon Europe Requirements (FAIR principles)
Metadata	Key words: biochar, ICP-OES, TGA, CHNS, ISO, surface area, particle size, volatile matter, ash content, dielectric analysis.
Tools for reuse	N/A
Data security	The data generated are stored with online and offline backups.
Data management cost	¼ PM
Accessibility & data sharing	Public
Copyright & IP management	None
Ethical issues management	In compliance with EU Regulation 2016/679 GDPR

Additional data management procedures	N/A
Related publication/s	None

Dataset ID	MOJITO_WP2_T2.3_pre_calcination_mixture_1.0
Task title	Task 2.3 Feedstock pretreatment, pre-calcination mixture preparation and characterization
Dataset name	Chemical and physical analysis of pre-calcination mixture
Ready at month of project	M12
Status	To start
Chosen Repository	NOMAD
PID [PID type]	DOI
Version	1
Task & data manager	UNIBO
Name of other partners involved	None
Creator/s	Melandri Marco [UNIBO-TPU]
Contributor/s	Antonio Primante [UNIBO-TPU], Alessia Alcantarini [UNIBO-TPU], Lucio Quadrani [UNIBO-TPU]
Contact Person/s	Melandri Marco [UNIBO-TPU, marco.melandri9@unibo.it]
Dataset description	This dataset contains information about dielectric analysis of carbonaceous materials grounded and screened at different grain sizes (500, 250, 180, 90, µm) and its change as function of the average size of the particles and of the temperature. This dataset contains dielectric analysis of the PCM:dolomite mixture 3:97, 6:94, 9:91, 12:88 in the range between 25 and 800 °C.
Data format	N/A
Data volume	N/A
Data handling standards	Data collection, aggregation, storage and sharing in compliance with Horizon Europe Requirements (FAIR principles)
Metadata	Key words: biochar, grain size, dielectric analysis, PCM:dolomite mixture
Tools for reuse	N/A
Data security	The data generated are stored with online and offline backups.
Data management cost	¼ PM
Accessibility & data sharing	Controlled access (username and password)
Copyright & IP management	CC-BY
Ethical issues management	In compliance with EU Regulation 2016/679 GDPR
Additional data management procedures	N/A
Related publication/s	None

Dataset ID	MOJITO_WP2_T2.4_calcinated_mixture_1.0
Task title	Task 2.4 Characterization of the material produced in rotary kiln calcination test
Dataset name	Chemical and physical analysis of calcined mixture
Ready at month of project	M32
Status	To start
Chosen Repository	NOMAD
PID [PID type]	DOI
Version	1
Task & data manager	UNIBO
Name of other partners involved	None
Creator/s	Melandri Marco [UNIBO-TPU]
Contributor/s	Antonio Primante [UNIBO-TPU], Alessia Alcantarini [UNIBO-TPU], Lucio Quadrani [UNIBO-TPU]
Contact Person/s	Melandri Marco [UNIBO-TPU, marco.melandri9@unibo.it]
Dataset description	This dataset contains analysis results of the calcined mixtures of carbonaceous and carbonate from T3.2 and 3.3. The analysis results include the concentrations of Na, K, Mg, Ca, Al, Si, P, Fe and heavy metals such as Pb, As, and Cd determined with ICP-OES; results from TGA and elemental analysis carried out using CHNS; surface area determined with physisorption; dielectric loss (ε") along with permittivity (ε') measured with a dielectric probe; data from XRD analysis; data from particle size, bulk density, free water, LOI 1050 and %CaO and %MgO ensuring compliance with UNI EN 459-2:2021.
Data format	N/A
Data volume	N/A
Data handling standards	Data collection, aggregation, storage and sharing in compliance with Horizon Europe Requirements (FAIR principles)
Metadata	Key words: CaO, MgO, CaCO3, carbonate, ICP-OES, TGA, CHNS, XRD, UNI EN 459-2:2021, surface area, dielectric analysis
Tools for reuse	N/A
Data security	The data generated are stored with online and offline backups.
Data management cost	¼ PM
Accessibility & data sharing	Controlled access (username and password)
Copyright & IP management	CC-BY
Ethical issues management	In compliance with EU Regulation 2016/679 GDPR
Additional data management procedures	N/A
Related publication/s	None

Dataset ID	MOJITO_WP2_T2.4_energy_data_1.0
Task title	Task 2.4 Characterization of the material produced in rotary kiln calcination test
Dataset name	Energy data
Ready at month of project	M32
Status	To start
Chosen Repository	NOMAD
PID [PID type]	DOI
Version	1
Task & data manager	UNIBO
Name of other partners involved	None
Creator/s	Melandri Marco [UNIBO-TPU]
Contributor/s	Antonio Primante [UN UNIBO-TPU IBO], Alessia Alcantarini [UNIBO-TPU], Lucio Quadrani [UNIBO-TPU]
Contact Person/s	Melandri Marco [UNIBO-TPU, marco.melandri9@unibo.it]
Dataset description	This dataset contains energy data from different energy supply configurations provided by the different electric/MW heating systems tested.
Data format	N/A
Data volume	N/A
Data handling standards	Data collection, aggregation, storage and sharing in compliance with Horizon Europe Requirements (FAIR principles)
Metadata	Key words: energy supply, heating system
Tools for reuse	N/A
Data security	The data generated are stored with online and offline backups.
Data management cost	¼ PM
Accessibility & data sharing	Controlled access (username and password)
Copyright & IP management	CC-BY
Ethical issues management	In compliance with EU Regulation 2016/679 GDPR
Additional data management procedures	N/A
Related publication/s	None

Dataset ID	MOJITO_WP2_T2.5_model_1.0
Task title	Task 2.5 Performance Measurements
Dataset name	Mass-energy balance data model
Ready at month of project	M36
Status	To start
Chosen Repository	NOMAD
PID [PID type]	DOI
Version	1
Task & data manager	UNIBO
Name of other partners involved	None
Creator/s	Melandri Marco [UNIBO-TPU]
Contributor/s	Antonio Primante [UNIBO-TPU], Alessia Alcantarini [UNIBO-TPU], Lucio Quadrani [UNIBO-TPU]
Contact Person/s	Melandri Marco [UNIBO-TPU, marco.melandri9@unibo.it]
Dataset description	This dataset contains data of energy intensity, carbon intensity, calcination rate, CO2 capture effectiveness in relation to the experimental conditions. Weight measurements, power measurements together with material characterisation data used to build a parametric mass-energy balance model that enables to anticipate the performance of the technology and its scale-up.
Data format	N/A
Data volume	N/A
Data handling standards	Data collection, aggregation, storage and sharing in compliance with Horizon Europe Requirements (FAIR principles)
Metadata	Key words: energy intensity, carbon intensity, calcination rate, CO2 capture, material characterisation, mass-energy balance
Tools for reuse	N/A
Data security	The data generated are stored with online and offline backups.
Data management cost	¼ PM
Accessibility & data sharing	Controlled access (username and password)
Copyright & IP management	CC-BY
Ethical issues management	In compliance with EU Regulation 2016/679 GDPR
Additional data management procedures	N/A
Related publication/s	None

Dataset ID	MOJITO_WP2_T3.1_pilot_plant_1.0
Task title	Task 3.1 Electric/MW rotary kiln choice, purchase and commissioning
Dataset name	Pilot-Plant
Ready at month of project	***18***
Status	Not yet available
Chosen Repository	NOMAD
PID [PID type]	DOI
Version	1.0
Task & data manager	Meiller, Martin [FRA]
Name of other partners involved	
Creator/s	Seeger, Jan [FRA]; Meiller, Martin [FRA]
Contributor/s	Seeger, Jan [FRA]; Meiller, Martin [FRA]; Primante Antonio [UNIBO]
Contact Person/s	Seeger, Jan [FRA, jan.seeger@umsicht.fraunhofer.de]; Meiller, Martin [FRA, Martin.Meiller@umsicht.fraunhofer.de]
Dataset description	This dataset compiles the calcination pilot plant engineering documentation—plant schematics, PFDs and P&IDs, general arrangement and mechanical drawings, electrical single-line diagrams, and vendor technical datasheets for major components. Files are provided as finalized PDFs with native CAD files (DWG/STEP) where available, plus CSV/Excel tables for calibration and parts lists. The documentation records design parameters (line sizes, materials, design pressures/temperatures), performance data and certificates from vendors, and calibration records.
Data format	PDF, Excel, Text-file
Data volume	5 GB
Data handling standards	Data collection, aggregation, storage and sharing in compliance with Horizon Europe Requirements (FAIR principles)
Metadata	Key words: calcination, carbon intensity, calcination rate, CO2 capture, material characterisation, mass-energy balance
Tools for reuse	Adobe Reader, Microsoft Excel
Data security	The data generated are stored with online and offline backups.
Data management cost	¼ PM
Accessibility & data sharing	A part of the Data will be publicly available especially Data sets of Experiments and DOE Data. Drawings and part lists of the Pilot plans are IP of third party and can thereby not be made openly available.
Copyright & IP management	All rights to the publicly available data will remain with Fraunhofer UMSICHT and the University of Bologna.
Ethical issues management	In compliance with EU Regulation 2016/679 GDPR
Additional data management procedures	N/A
Related publication/s	None

Dataset ID	MOJITO_WP3_T3.4_COMSOL_1.0
Task title	Task 3.4 Multiphysics model of the rotary kiln
Dataset name	COMSOL model
Ready at month of project	***20***
Status	Not yet available
Chosen Repository	NOMAD
PID [PID type]	DOI
Version	1.0
Task & data manager	Antonio Primante [UNIBO-TPU]
Name of other partners involved	
Creator/s	Alessia Alcantarini [UNIBO-TPU], Lucio Quadrani [UNIBO-TPU]
Contributor/s	
Contact Person/s	
Dataset description	COMSOL dataset of calcination simulations: time-dependent 1D/2D/3D models coupling heat transfer, mass transport, reaction kinetics and phase change to capture temperature, CO_2 release, conversion and porosity evolution under varied operating conditions. The archive contains .mph model files, parameter tables (CSV/JSON), exported results (VTK/CSV/.mat), Python/MATLAB postprocessing scripts, and per-run metadata for material properties, Arrhenius kinetics, mesh/time-step settings and validation (TG/DTA comparisons and convergence tests where available).
Data format	COMSOL-Modelfile (.mph)
Data volume	25 GB
Data handling standards	Data collection, aggregation, storage and sharing in compliance with Horizon Europe Requirements (FAIR principles)
Metadata	Key words: CaO, MgO, CaCO3, carbonate, calcination, simulation
Tools for reuse	COMSOL Multiphysics
Data security	The data generated are stored with online and offline backups.
Data management cost	¼ PM
Accessibility & data sharing	Controlled access (username and password)
Copyright & IP management	All rights to the publicly available data will remain with FRA and UNIBO.
Ethical issues management	none
Additional data management procedures	N/A
Related publication/s	Not known yet

Dataset ID	MOJITO_WP4_T4.1_DFT-NEB_1.0
Task title	Task 4.1 First-principles prediction of the activation energies and reaction paths of the calcination process
Dataset name	DFT-NEB_dataset
Ready at month of project	M9
Status	In progress
Chosen Repository	NOMAD
PID [PID type]	DOI
Version	V_1
Task & data manager	UNIBO, Maria Clelia Righi
Name of other partners involved	
Creator/s	Maria Patanè [UNIBO-CMU]
Contributor/s	Maria Patanè, Paolo Restuccia, Maria Clelia Righi [UNIBO-CMU]
Contact Person/s	Maria Clelia Righi [UNIBO-CMU] clelia.righi@unibo.it
Dataset description	The dataset consists of *ab initio* computational data generated to study the calcination process at the atomistic level. It includes self-consistent field (SCF) calculations and Nudged Elastic Band (NEB) simulations used to determine reaction pathways and activation energies, in line with the objectives of the MOJITO project. Quality assurance is ensured by using validated computational codes, standardized convergence criteria, and consistency checks against literature results. The dataset may be useful outside the project to researchers in computational materials science as reference data for reaction mechanisms and energy barriers. Although similar first-principles results exist in the literature, the raw data are not available and therefore cannot be used. Consequently, dedicated simulations were necessary to achieve the project objectives.
Data format	The input and output files, which are plain-text files written in Quantum ESPRESSO namelist format, will be archived in NOMAD, where JSON files will also be produced.
Data volume	1 GB
Data handling standards	No specific disciplinary standards apply; the data generated are manually stored
Metadata	Metadata will be present as encoded in NOMAD Metainfo, which contains specific schemes for computational data https://nomad-lab.eu/prod/v1/docs/examples/computational_data/metainfo.html
Tools for reuse	The provided Input files will allow anyone to re-calculate the data by means of the open-source programs used to generate the data. The details of the adopted methodology, data analysis will be described in the deliverable report and published papers.
Data security	The data generated are stored with online and offline backups.
Data management cost	1/4 PM
Accessibility & data sharing	The data will be made openly available after an embargo period of 3–6 months following submission or immediately upon publication of the associated paper.
Copyright & IP management	CC-BY
Ethical issues management	None
Additional data management procedures	N/A
Related publication/s	

Dataset ID	MOJITO_WP4_T4.2_MLFF_1.0
Task title	Task T4.2 MLFFs development
Dataset name	MLFFs_Dataset
Ready at month of project	M18
Status	In progress
Chosen Repository	NOMAD
PID [PID type]	DOI
Version	V_1
Task & data manager	UNIBO, Maria Clelia Righi
Name of other partners involved	
Creator/s	Maria Patanè [UNIBO-CMU]
Contributor/s	Maria Patanè, Paolo Restuccia, Maria Clelia Righi [UNIBO-CMU]
Contact Person/s	Maria Clelia Righi [UNIBO-CMU] clelia.righi@unibo.it
Dataset description	The generation of machine-learning force fields (MLFFs) is required to accurately describe atomistic interactions in the materials present in the rotary kiln. The starting point for training the MLFFs will be the first principles calculations performed in Task 4.1. Since this initial dataset will be quite limited, we will enrich it by sampling a larger area of the configuration space through an active learning approach as implemented in the SCS code developed by the UNIBO-CMU. This approach enables the construction of reliable force fields with high accuracy at a reduced computational cost, making the methodology accessible and useful also to researchers outside the project and to the best of our knowledge, is not currently available in the literature.
Data format	The input and output files, which are plain-text files, will be archived in NOMAD, where JSON files will also be produced.
Data volume	1 GB
Data handling standards	No specific disciplinary standards apply; however, the data generated are manually stored
Metadata	Metadata will be present as encoded in NOMAD Metainfo, which contains specific schemes for computational data https://nomad-lab.eu/prod/v1/docs/examples/computational_data/metainfo.html
Tools for reuse	The provided Input files will allow anyone to re-calculate the data by means of the open-source programs used to generate the data. The details of the adopted methodology, data analysis will be described in the deliverable report and published papers.
Data security	The data generated are stored with online and offline backups.
Data management cost	1/4 PM
Accessibility & data sharing	The data will be made openly available after an embargo period of 3–6 months following submission or immediately upon publication of the associated paper.
Copyright & IP management	CC-BY
Ethical issues management	None
Additional data management procedures	N/A
Related publication/s	None

Dataset ID	MOJITO_WP4_T4.2_microwave_absorption_1.0
Task title	Task 4.2 Modelling microwave absorption in PCMs
Dataset name	Microwave_absorption_simulation_data
Ready at month of project	M18
Status	In progress
Chosen Repository	NOMAD
PID [PID type]	DOI
Version	
Task & data manager	UNIBO, Maria Clelia Righi
Name of other partners involved	
Creator/s	Lucrezia Berghenti [UNIBO-CMU]
Contributor/s	Lucrezia Berghenti, Margherita Marsili, Maria Clelia Righi [UNIBO-CMU]
Contact Person/s	Maria Clelia Righi [UNIBO-CMU] clelia.righi@unibo.it
Dataset description	This dataset collects data generated by first principles simulations of graphene flakes dielectric functions including both the electronic and vibrational contributions. It includes relaxed geometries, electronic structures and dielectric functions of graphene flakes whose size, geometry and functionalization has been systematically varied in line with the project of objective of identifying the optimal configuration for enhanced MW absorption. To the best of our knowledge, such systematic analysis is not available yet, and these data might be useful for researchers interested in tailoring the electronic and optical properties of this class of materials. The quality of the data is assessed by the use of validated computational codes and standardized convergence tests against all relevant computational parameters.
Data format	
Data volume	1 GB
Data handling standards	No specific disciplinary standards apply; however, the data generated are manually stored
Metadata	
Tools for reuse	
Data security	The data generated are stored with online and offline backups.
Data management cost	
Accessibility & data sharing	The data will be made openly available after an embargo period of 3–6 months following submission or immediately upon publication of the associated paper.
Copyright & IP management	CC-BY
Ethical issues management	None
Additional data management procedures	N/A
Related publication/s	

Dataset ID	MOJITO_WP4_T4.4_MD_simulation_1.0
Task title	Task 4.4 MD simulations of the calcination process in vacuum
Dataset name	MD_simulation_calcination_Dataset
Ready at month of project	M30
Status	In progress
Chosen Repository	NOMAD
PID [PID type]	DOI
Version	V_1
Task & data manager	UNIBO, Maria Clelia Righi
Name of other partners involved	
Creator/s	Maria Patanè [UNIBO-CMU]
Contributor/s	Maria Patanè, Paolo Restuccia, Maria Clelia Righi [UNIBO-CMU]
Contact Person/s	Maria Clelia Righi [UNIBO-CMU] clelia.righi@unibo.it
Dataset description	This dataset contains results from ML-MD simulations of the $CaCO_3$ calcination process under vacuum conditions. The simulations are designed to uncover the atomistic mechanisms underlying the calcination reaction, providing detailed insight into bond breaking and formation, structural evolution, and reaction pathways at the atomic scale that are not available in the existing literature.
Data format	The input and output files, which are plain-text files, will be archived in NOMAD, where JSON files will also be produced.
Data volume	1 GB
Data handling standards	No specific disciplinary standards apply; however, the data generated are manually stored
Metadata	Metadata will be present as encoded in NOMAD Metainfo, which contains specific schemes for computational data https://nomad-lab.eu/prod/v1/docs/examples/computational_data/metainfo.html
Tools for reuse	The provided Input files will allow anyone to re-calculate the data by means of the programs used to generate the data. The details of the adopted methodology, data analysis will be described in the deliverable report and published papers.
Data security	The data generated are stored with online and offline backups.
Data management cost	¼ PM
Accessibility & data sharing	The data will be made openly available after an embargo period of 3–6 months following submission or immediately upon publication of the associated paper.
Copyright & IP management	CC-BY
Ethical issues management	None
Additional data management procedures	N/A
Related publication/s	None

Annex II: Open Access status of project publications

No project publications yet.

Annex III: "README" file template

A "README" file is a document that will be deposited with each dataset, containing relevant information about dataset authorship, terms of reuse and responsibilities, explaining dataset content and structure, collection procedures and analysis (such as file specifics, methodologies, codebooks of variables, data sources, and further necessary notes).
In the following there is a template of the README file that we will use.

README file

Dataset Title: "[insert title as defined in the DMP]"
Dataset Author/s: Name Surname (Affiliation), ORCID (if available);
Dataset Contributor/s: Name Surname (Affiliation), ORCID (if available);
Dataset Contact Person/s: Name Surname (Affiliation), ORCID (if available), email;
Dataset License: this dataset is distributed under a [insert LICENSE]
Publication Year: [insert YEAR]
Project Info: Mojito Decarbonized Lime Production Through Enhanced Joint Dielectric Heating and Waste Carbonaceous Material Addition, funded by European Union, EIC-2024-PathfinderChallenges. Grant Agreement num. 101221957; www.mojito-project.eu

Dataset Contents

The dataset consists of:
EXAMPLE 1

- 1 textual qualitative file saved in .rtf format: "MOJITO_WPn_Tn.m_[description]_[yyyymmdd]_v01.rtf"
- 1 README file: "README_ MOJITO_WPn_Tn.m_[description]_[yyyymmdd]_v01.rtf"

EXAMPLE 2

- 1 tabular quantitative file saved in .csv format: "MOJITO_WPn_Tn.m_[description]_[yyyymmdd].csv"
- 1 README file: "README_ MOJITO_WPn_Tn.m_[description]_[yyyymmdd].txt"]

Dataset Documentation

Abstract:
[Insert dataset abstract]
Content of the files:

- file [Insert filename] contains ...
- file [Insert filename] contains ...
- …

File specifics
[Please indicate instruction/technical info in order to allow potential users to correctly visualize and reuse your data (e.g. specific software, …). In case of data converted in open formats it could be useful to provide some further information. For example, if you deposit for long term preservation a .csv file derived from an excel you can describe the conversion. Here is an example of description of conversion using libre office calc software:
To create the .csv files, "LibreOffice Calc" version: n.m.p.q (portable) was used, with the following specifics:
•Character set Europa occidentale (Windows-1252/WinLatin1)
•Field delimiter « , » (comma)
•Text delimiter « " » (quotes)]
Notes
[Related to the whole dataset or to single files of a multi-file dataset (Optional)]
Data sources
[Optional]
Methodologies
[If necessary to understand how to reuse data]
Codebook of variables
[If necessary to understand the meaning of the variables]