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# KINETIC MODELING OF VERY LOW CLINKER CEMENTS

*A Data Management Plan created using DMPonline.be*

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**Template:** KU Leuven BOF-IOF

**Grant number / URL:** C2E/23/003

**ID:** 202531

**Start date:** 01-10-2023

**End date:** 30-09-2027

**Project abstract:**

High-level replacement of clinker by supplementary cementitious materials (SCMs) offers a well-tried solution to reducing CO<sub>2</sub> emissions of cement production. To sustain further clinker reductions, new sources and combinations of SCMs will need to step in and their impact on cement hydration will need to be understood by comprehensive hydration models. A key input for cement hydration models, whether based on thermodynamic, microstructural, or simple mass balance principles, are time-dependent data on reaction degrees of all cement constituents. At present kinetic models that capture and describe reaction kinetics of SCMs are lacking, in particular for cements with very low clinker (VLC) contents. To overcome this gap, the VLC project aims to develop a new kinetic model for SCM reactivity feeding on a broad reactivity database. By combination with thermodynamic and microstructural modelling codes, this new kinetic model will enable exploration and prediction of the impact of SCM reactions on the cement hydrate assemblage, microstructure and eventually, performance as well as fostering the development of the next generation of very low carbon cements.

**Last modified:** 27-10-2023

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## Research Data Summary

List and describe all datasets or research materials that you plan to generate/collect or reuse during your research project. For each dataset or data type (observational, experimental etc.), provide a short name & description (sufficient for yourself to know what data it is about), indicate whether the data are newly generated/collected or reused, digital or physical, also indicate the type of the data (the kind of content), its technical format (file extension), and an estimate of the upper limit of the volume of the data.

Dataset name / ID	Description	New or reuse	Digital or Physical data	Data Type	File format	Data volume	Physical volume
		Indicate: <b>N</b> (ew data) or <b>E</b> (xisting data)	Indicate: <b>D</b> (igital) or <b>P</b> (hysical)	Indicate: <b>A</b> udiovisual <b>I</b> mages <b>S</b> ound <b>N</b> umerical <b>T</b> extual <b>M</b> odel <b>S</b> oftware Other (specify)		Indicate: <1GB <100GB <1TB <5TB >5TB NA	
1. Reactivity dataset	Database of reactivity test data (various tests)	N and E	D	N	.csv	<10GB	-
2. Material characterisation database	Database collecting all test material properties (composition, physical properties,...)	N and E	D and P	N	.csv	<1GB	50-100 specimens (100-200 g each)
3. Kinetic model	Modelling platform/code for reactivity of SCMs	N	D	M	python	<1GB	
4. Cement hydration studies	Experimental data on SCM reactivity in VLC cements	N	D	N	.csv	<10GB	
5. Thermodynamic modelling results	Modelling results (composition, energy landscape)	N	D	N	.csv	<1GB	
6. Data on mechanical and sustainability performance of VLC cements	Experimental and calculation data on performance characteristics (strength, durability, sustainability)	N	D	N	.csv	<1GB	

If you reuse existing data, please specify the source, preferably by using a persistent identifier (e.g. DOI, Handle, URL etc.) per dataset or data type:

Data presented in following publications will be reused as part of the project database:

- <https://doi.org/10.1617/s11527-022-01947-3>
- <https://doi.org/10.1617/s11527-022-01928-6>
- <https://doi.org/10.1617/s11527-018-1269-x>

Are there any ethical issues concerning the creation and/or use of the data (e.g. experiments on humans or animals, dual use)? If so, refer to specific datasets or data types when appropriate and provide the relevant ethical approval number.

- No

Will you process personal data? If so, please refer to specific datasets or data types when appropriate and provide the KU Leuven or UZ Leuven privacy register number (G or S number).

- No

Does your work have potential for commercial valorization (e.g. tech transfer, for example spin-offs, commercial exploitation, ...)? If so, please comment per dataset or data type where appropriate.

- Yes

The economic return will largely result from follow-up R&D projects and delivery of consultancy services based on the kinetic modelling framework developed in the project. The model will enable to capture data from the recently developed and standardised R3 test method in order to grow the database and further improve and extend its predictive performance. When validated and fully operational the VLC kinetic model can be built in or linked to existing codes or software that will upscale the reaction kinetics modelling output to macroscopic performance or durability properties of concrete elements or structures.

Do existing 3rd party agreements restrict exploitation or dissemination of the data you (re)use (e.g. Material or Data transfer agreements, Research collaboration agreements)? If so, please explain in the comment section to what data they relate and what restrictions are in place.

- Yes

Part of the published data to be used in the project can only be used pseudonymised, i.e. the source and supplier of the materials cannot be disclosed.

**Are there any other legal issues, such as intellectual property rights and ownership, to be managed related to the data you (re)use? If so, please explain in the comment section to what data they relate and which restrictions will be asserted.**

- No

## Documentation and Metadata

**Clearly describe what approach will be followed to capture the accompanying information necessary to keep data understandable and usable, for yourself and others, now and in the future (e.g. in terms of documentation levels and types required, procedures used, Electronic Lab Notebooks, README.txt files, codebook.tsv etc. where this information is recorded).**

We will use an excel file to log and capture documentation accompanying (sets of) measurements, code, simulation results.

For measurement data (datasets 1, 2, 4, 6) following information will be typically included: - Name of file or dataset

- Project name
- Date of creation/measurement
- Name and contact information of author
- Name and contact information of Principal Investigator
- Description of the dataset, sample information
- Number of files included
- List with names of files, description, date of creation
- File Formats
- Software used to generate data
- Software needed to open files
- Naming convention for file names
- Storage location(s)
- Aim for which the data were collected - reference to experiment design form
- Data collection method, instrument, instrument settings
- Data processing method, software, model
- Recommended citation for the dataset
- Confidentiality information
- Full names and definitions for column and rows
- Explanation of abbreviations
- Units of measurement
- Publications based on this dataset
- Relationship to other datasets
- References of publications used to create the dataset

For modelling code (dataset 3) following information will be typically included:

- Name of file or dataset
- Project name
- Date of creation/measurement
- Name and contact information of author
- Name and contact information of Principal Investigator
- Description of the code
- Number of files included
- List with names of files, description, date of creation
- File Formats
- Software used to develop the code
- Software needed to run the code
- Naming convention for file names
- Storage location(s)
- Aim for which the code was developed
- Data processing method, software, model
- Recommended citation for the code
- Confidentiality information
- Explanation of abbreviations
- Units
- Publications based on this code
- Relationship to other codes
- References of publications used to create the code

For simulation results (dataset 5, 6) following information will be typically included:

- Name of file or dataset
- Project name
- Date of creation/measurement
- Name and contact information of author
- Name and contact information of Principal Investigator
- Description of the dataset, simulation information
- Number of files included
- List with names of files, description, date of creation
- File Formats
- Software used to generate data
- Software needed to open files
- Naming convention for file names
- Storage location(s)

- Aim for which the data were collected
- Recommended citation for the dataset
- Confidentiality information
- Full names and definitions for column and rows
- Explanation of abbreviations
- Units of measurement
- Publications based on this dataset
- Relationship to other datasets
- References of publications used to create the dataset

**Will a metadata standard be used to make it easier to find and reuse the data?**

**If so, please specify which metadata standard will be used.**

**If not, please specify which metadata will be created to make the data easier to find and reuse.**

- Yes

The KU Leuven RDR metadata standard DataCite will be used.

## Data Storage & Back-up during the Research Project

**Where will the data be stored?**

- OneDrive (KU Leuven)
- Sharepoint online

During the project data will be stored in a MS TEAMS project platform. This Teams platform is structured for collaboration, sharing and storage of data.

**How will the data be backed up?**

- Standard back-up provided by KU Leuven ICTS for my storage solution

**Is there currently sufficient storage & backup capacity during the project?**

**If no or insufficient storage or backup capacities are available, explain how this will be taken care of.**

- Yes

**How will you ensure that the data are securely stored and not accessed or modified by unauthorized persons?**

The TEAMS sharepoint is only made accessible to the research team members. Access is given by the project coordinator.

**What are the expected costs for data storage and backup during the research project? How will these costs be covered?**

At this stage, KU Leuven centrally covers the costs related to data storage and backup of the TEAMS sharepoint.

## Data Preservation after the end of the Research Project

**Which data will be retained for 10 years (or longer, in agreement with other retention policies that are applicable) after the end of the project?**

**In case some data cannot be preserved, clearly state the reasons for this (e.g. legal or contractual restrictions, storage/budget issues, institutional policies...).**

- All data will be preserved for 10 years according to KU Leuven RDM policy

**Where will these data be archived (stored and curated for the long-term)?**

- Shared network drive (J-drive)
- KU Leuven RDR

All project data will be stored on the secured archiving drive maintained by the IT services of the Department of Earth and Environmental Sciences. Research data used in or supporting published manuscripts will be publicly shared by archiving in the KU Leuven Research Data Repository (RDR).

**What are the expected costs for data preservation during the expected retention period? How will these costs be covered?**

We expect that the total size of data will not exceed 500 GB, which is comprised within the MS TEAMS sharepoint without cost.

## **Data Sharing and Reuse**

**Will the data (or part of the data) be made available for reuse after/during the project?**

**Please explain per dataset or data type which data will be made available.**

- Yes, as open data
- Yes, as restricted data (upon approval, or institutional access only)

Datasets 1, 4, 5, 6 will be made openly available.

Dataset 2 (material characterisation) will be partially restricted due to prior material transfer agreements with suppliers.

Dataset 3 (kinetic modelling code) will be shared upon approval. The principle is to share the code only with trustable users/research teams.

**If access is restricted, please specify who will be able to access the data and under what conditions.**

Dataset 3 (kinetic modelling code) will be restricted and shared upon approval. The principle is to share the code only with trustable users/research teams upon concluding a developer or end-user agreement.

**Are there any factors that restrict or prevent the sharing of (some of) the data (e.g. as defined in an agreement with a 3rd party, legal restrictions)?**

**Please explain per dataset or data type where appropriate.**

- Yes, intellectual property rights

Dataset 1 (reactivity dataset) - existing data to be reused is publicly available under an open access agreement, moreover the research team was directly involved in the collection of these existing dataset.

Dataset 2 (material characterisation) will be partially restricted due to prior material transfer agreements with suppliers that prohibit disclosure of origin and supplier. Therefore only pseudonymized data will be shared.

Dataset 3 (kinetic modelling code) will be restricted and shared upon approval. We intend to make the first version(s) of the VLC kinetic model open and free to trustable end-users. This will raise interest from users and help building a user base.

**Where will the data be made available?**

**If already known, please provide a repository per dataset or data type.**

- KU Leuven RDR (Research Data Repository)
- Other data repository (specify below)

Research data used in or supporting published manuscripts will be publicly shared by archiving in the KU Leuven Research Data Repository (RDR). This may relate to all defined datasets.

We will define if also finished, yet unpublished data can be archived on KU Leuven RDR, or if other repositories are more suitable (e.g. dataset 3 - modelling code, through a more direct download link on the research group website in order to keep better track of versioning).

**When will the data be made available?**

- Upon publication of research results
- Specific date (specify below)

Finished, yet unpublished data will be made available latest 6 months after the end of the project, this time delay would allow for publication of late manuscripts.

**Which data usage licenses are you going to provide?**

**If none, please explain why.**

- CC-BY 4.0 (data)
- Data Transfer Agreement (restricted data)
- GNU GPL-3.0 (code)

**Do you intend to add a persistent identifier (PID) to your dataset(s), e.g. a DOI or accession number? If already available, please provide it here.**

- Yes, a PID will be added upon deposit in a data repository

**What are the expected costs for data sharing? How will these costs be covered?**

We don't expect additional costs as the total volume of finished datasets will likely not exceed 50 GB, which is in line with RDR free allowance.

**Responsibilities****Who will manage data documentation and metadata during the research project?**

The project PhD researchers are responsible for documentation of the data they generate, as well as providing adequate metadata.

PhD researcher 1 will document all experimental data collected in WP1 (Reactivity testing, hydration experiments,...), as well as the modelling algorithms, codes and results generated in WP2.

PhD researcher 2 will be responsible for documentation of data and metadata generated in WP3 (experimental data from cement hydration studies), WP4 (modelling results from thermodynamic modelling), as well as WP5 (performance validation - experimental data and sustainability calculations).

The KU Leuven supervisors will have end responsibility in terms of data documentation and will regularly verify if the data are properly documented.

**Who will manage data storage and backup during the research project?**

All researchers will be responsible for storage of the data they have generated on the project MS TEAMS sharepoint, following the structure and guidelines provided by the project coordinator.

The supervisors will verify adequate data storage.

The SET-IT KU Leuven team maintaining the MS TEAMS platform are responsible for daily back-ups of the data.

**Who will manage data preservation and sharing?**

WP1 and WP2 related data: Prof. Ruben Snellings

WP3, 4, 5: Prof. Özlem Cizer

**Who will update and implement this DMP?**

Prof. Ruben Snellings as project coordinator will have end responsibility for updating and implementing the DMP.