Pore-scale modelling of moisture transfer in building materials: full-scale pore network construction and hygric property simulation

A Data Management Plan created using DMPonline.be

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Template: FWO DMP (Flemish Standard DMP)

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Project Administrator: Hans Janssen

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Project abstract:

What if we were able to fully exploit the relation between the pore structure and the hygric properties of porous materials to truly 'engineer' the moisture performance of building materials? Or more specifically, what if we were able to predict the moisture properties of building materials directly from pore structure information? This would accelerate the hygric analysis of existing building materials and facilitate the hygric design of new building materials. In recent years, research by the "Transport in porous materials"

research group – of the Building Physics Section in the Department of Civil Engineering of KU Leuven – has made such numerical prediction of moisture properties of building materials based on pore structure possible. The full-blown application of such pore-scale modelling is hindered by two bottle-necks though: the generation of full-scale pore networks spanning the entire spectrum of pore sizes in building materials, and the computation of moisture properties in these full-scale pore networks. The project aims at taking pore-scale modelling of moisture properties of building materials to the next level, via full-scale stochastic generation of pore networks for building materials as well as proficient algorithms for moisture storage and transport simulation in these networks. The efficacy and reliability of pore-scale modelling of moisture properties of building materials is finally verified by validation with already available moisture properties.

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Questionnaire

Describe the datatypes (surveys, sequences, manuscripts, objects ...) the research will collect and/or generate and /or (re)use. (use up to 700 characters)

Various datatypes will be generated:

- material specimen for measurements: typically stored as physical objects;
- experimental protocols and outcomes: typically stored as computer objects, in text and spreadsheet formats as well as in dedicated image files;
- simulation models' inputs and outputs: typically stored as computer objects, in text and spreadsheet formats as well as in dedicated model files;
- publications (reports, papers, reviews): typically stored as computer objects, in text formats;

Specify in which way the following provisions are in place in order to preserve the data during and at least 5 years after the end of the research? Motivate your answer. (use up to 700 characters)

The responsible persons are the two Pl's, prof. Hans Janssen and prof. Stefan Vandewalle. Storage provisions and guidelines are in place, for physical objects (prof. Hans Janssen) as well as computer objects (prof. Hans Janssen & prof. Stefan Vandewalle).

These physical objects (material samples) will be stored in the laboratory storage room of the Building Physics and Sustainable Design section (Department of Civil Engineering) with clear marking of their origin, meaning, storage intent and required storage duration.

These computer files (text files, spreadsheet files, computer codes, ...) will be archived on the storage disks of both the Building Physics and Sustainable Design section (Department of Civil Engineering) and the Numerical Analysis and Applied Mathematics (NUMA) section (Department of Computer Sciences), typically used for archiving computer objects related to research activities.

What's the reason why you wish to deviate from the principle of preservation of data and of the minimum preservation term of 5 years? (max. 700 characters)

Not applicable

Are there issues concerning research data indicated in the ethics questionnaire of this application form? Which specific security measures do those data require? (use up to 700 characters)

Not applicable

Which other issues related to the data management are relevant to mention? (use up to 700 characters)

Not applicable

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1. 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.

Various datatypes will be generated:

- simulation models' inputs and outputs: typically stored as computer objects, in text and spreadsheet formats as well as in dedicated model files;
- publications (reports, papers, reviews): typically stored as computer objects, in text formats;

				Only for digital data	Only for digital data	Only for digital data	Only for physical data
Dataset Name	Description	New or reused	Digital or Physical	Digital Data Type	Digital Data format	Digital data volume (MB/GB/TB)	Physical volume
	Material samples used for characterisation of the pore structure of three building materials	Generate new data	Physical	Experimental	Not applicable	Not applicable	< 0.1 m ³
Protocols	Protocols for execution of characterisation experiments	Generate new data	Digital	Documentation	.txt, .cvs, .pdf	< 100MB	Not applicable
Outcomes	Outcomes of execution of characterisation experiments	Generate new data		Experimental & Compiled/aggregated	.txt, .cvs, .pdf, .tif	< 1TB	Not applicable
livioneis	Pore network extraction, generation and simulation computer models	Generate new data	Digital	Software	.py, .pyi, .pyc, .pyd, .pyo, .pyw, .pyz, .txt, .cvs, .pdf	< 1GB	Not applicable
Publications	Reports, papers, reviews on all aspects of the research	Generate new data	Digital	Documentation	.txt, .cvs, .pdf	< 1GB	Not applicable

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:

Not applicable

Are there any ethical issues concerning the creation and/or use of the data (e.g. experiments on humans or animals, dual use)? Describe these issues in the comment section. Please refer to specific datasets or data types when appropriate.

No

Will you process personal data? If so, briefly describe the kind of personal data you will use in the comment section. Please refer to specific datasets or data types when appropriate.

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.

No

Do existing 3rd party agreements restrict exploitation or dissemination of the data you (re)use (e.g. Material/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.

• No

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

2. 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).

A ReadMe file (.txt) can be found in the respective folders for each the different data sets, describing the actual content, overall organisation and further documentation of the stored data. This ReadMe file may also contains references to other documents with more details on certain elements (e.g. experimental protocols, post-processing procedures, simulation manuals, ...). The structure of every ReadMe file is based on the example documentation provided by the KU Leuven (https://www.kuleuven.be/rdm/en/README). Its template is also kept in the central folder of the project to make sure it can always be accessed.

Will a metadata standard be used to make it easier to find and reuse the data? If so, please specify (where appropriate per dataset or data type) which metadata standard will be used. If not, please specify (where appropriate per dataset or data type) which metadata will be created to make the data easier to find and reuse.

No

See above

3. Data storage & back-up during the research project

Where will the data be stored?

Depending on their size (and the costs involved), the data will be stored on either Shared Network Drive or Large Volume Storage, both provided by KU Leuven.

How will the data be backed up?

KU Leuven has proper protocols in place for backing up the Shared Network Drive or Large Volume Storage.

Is there currently sufficient storage & backup capacity during the project? If yes, specify concisely. If no or insufficient storage or backup capacities are available, then explain how this will be taken care of.

• Yes

The volumes of digital data to be stored are not excessive, and KU Leuven offers sufficient space via Shared Network Drive or Large Volume Storage.

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

KU Leuven has proper protocols in place to securely store digital data, avoiding access by unauthorized persons.

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

The volumes of digital data to be stored are not excessive, and the costs incurred are thus not very signficant. They are covered by the working budgets of the two sections involved.

4. Data preservation after the end of the research project

Which data will be retained for at least five 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, in accordance with KU Leuven's RDM policy.

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

Depending on their size (and the costs involved), the data will be stored on either Shared Network Drive or Large Volume Storage, both provided by KU Leuven.

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

The volumes of digital data to be stored are not excessive, and the costs incurred are thus not very signficant. They are covered by the working budgets of the two sections involved.

5. Data sharing and reuse

Will the data (or part of the data) be made available for reuse after/during the project? In the comment section please explain per dataset or data type which data will be made available.

• Yes, in a restricted access repository (after approval, institutional access only, ...)

All data will be made available, upon mailed request to the PI's.

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

The data will be available for reuse by other researchers within the two research groups involved. Everything can be retrieved from the archive drives of the research groups.

Researchers from outside the research group can request specific data via mailed request to the PI's.

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 in the comment section per dataset or data type where appropriate.

No

Not applicable

Where will the data be made available? If already known, please provide a repository per dataset or data type.

The data will be available for reuse by other researchers within the two research groups involved. Everything can be retrieved from the archive drives of the research groups.

Researchers from outside the research group can request specific data via mailed request to the PI's.

When will the data be made available?

Immediately after the end of the project

Which data usage licenses are you going to provide? If none, please explain why.

- for data (excluding software source code): CC-BY-NC-SA-4.0
- for software source code: AGPL-3.0-or-later

Do you intend to add a PID/DOI/accession number to your dataset(s)? If already available, you have the option to provide it in the comment section.

No

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

The volumes of digital data to be stored are not excessive, and the costs incurred are thus not very signficant. They are covered by the working budgets of the two sections involved.

6. Responsibilities

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

The related researchers: Chengnan Shi & TBD, under supervision of the Pl's: Hans Janssen & Stefan Vandewalle

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

The related researchers: Chengnan Shi & TBD, under supervision of the PI's: Hans Janssen & Stefan Vandewalle

Who will manage data preservation and sharing?

The related researchers: Chengnan Shi & TBD, under supervision of the Pl's: Hans Janssen & Stefan Vandewalle

Who will update and implement this DMP?

The related researchers: Chengnan Shi & TBD, under supervision of the Pl's: Hans Janssen & Stefan Vandewalle

Pore-scale modelling of moisture transfer in building materials: full-scale pore network construction and hygric property simulation GDPR

GDPR

Have you registered personal data processing activities for this project?

• Not applicable

Pore-scale modelling of moisture transfer in building materials: full-scale pore network construction and hygric property simulation DPIA

DPIA

Have you performed a DPIA for the personal data processing activities for this project?

• Not applicable

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