Energy-efficient gas drying with thermo-responsive desiccants

A Data Management Plan created using DMPonline.be

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Project abstract:

Many industrial processes make use of dry gases, especially dry air. The state-of-the-art technologies are active cooling to provoke condensation of water vapor and adsorption using desiccants. Active cooling is done by cooling below the dew point temperature causing supersaturation and condensation. Its use is appropriate for treating high relative humidity air. Desiccant technologies are more popular because they allow for deeper drying. The regeneration of conventional adsorbent needs to be done thermally at 150-250°C and is very energy demanding. Drying of air and industrial gases is responsible for ca. 15% of the energy consumption in the chemical industry. We propose research into a much more energy efficient technology, expected to reduce the energy demand with 60%. Thermo-responsive desiccants are switching from hydrophilic to hydrophobic with temperature. Water vapor is absorbed at low temperature and released in liquid form upon heating above the hydrophilicity switching temperature. This temperature typically is around 40-80°C making it very attractive for using even waste heat for the regeneration step. This polymer technology has been developed in the biomedical field for drug delivery applications. Here an application in the chemical industry is proposed. The research focus will be toward mastering the physico-chemical properties of the polymer to maximize water removal. We introduce a new concept of "osmocapillary" condensation in a thermo-responsive polymer.

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Energy-efficient gas drying with thermo-responsive desiccants Application DMP

Questionnaire

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

- 1. Experimental data of polymer synthesis
- 2. Polymer samples (WP1)
- 3. Characterization data of materials (SEM, EDX, N2 physisorption, NMR) (WP1)
- 4. Evaluation of materials' performance (WP2 & WP3)

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)

1. Designation of responsible person (If already designated, please fill in his/her name.)

Responsible person during the research: Anke Snauwaert

Responsible person after finishing of the research project: Johan Martens

- 2. Storage capacity/repository
 - during the research
 - o after the research

The required storage for data resulting from the research project is relatively small, the standard storage provided by the university suffices.

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)

I do not wish to deviate. Data will be preserved for at least 10 years, conform the KU Leuven RDM policy.

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)

No.

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

Not applicable.

Energy-efficient gas drying with thermo-responsive desiccants FWO DMP (Flemish Standard DMP)

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.

				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
		Please choose from the following options: Generate new data Reuse existing data	Please choose from the following options: • Digital • Physical	Compiled/aggregated dataSimulation data	Please choose from the following options: • .por, .xml, .tab, .csv,.pdf, .txt, .rtf, .dwg, .gml,	Please choose from the following options: • <100MB • <1GB • <100GB • <1TB • <5TB • <10TB • <50TB • <50TB • NA	
1. Experimental data of polymer synthesis (WP 1)	Data on composition of different polymer materials.	Generate new data	Digital	Experimental data	.xls		
2. Polymer samples (WP 1)	Physical samples synthesized during the research project.	Generate new data	Physical	Physical data			< 5 g of each sample
3. Characterization data of materials (SEM, EDX, N2 fysisorption, NMR) (WP 1)	samples,	Generate new data	Digital	Experimental data	.xls .tif	< 100 GB	
4. Evaluation of materials performance (WP 2 & WP 3)	Data generated by evaluation of the polymer samples, obtained by instruments	Generate new data	Digital	Experimental data	.xls	< 100 GB	

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:

No existing data is used.

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.
• Yes
Before publication of relevant data, there will be checked whether the data is patentable to protect the data with view on potential commercial exploitation.
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).
Polymer materials will be named after the date they are synthesized on (e.g. 010124 = synthesis on the first of January 2024). All data

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.

considering the synthesis (procedure, concentrations,...) and characterization (SEM, N2 physisorption,...) will be stored using this same system. An overview of all samples synthesized (including a short description) and characterizations carried out on these samples is kept in an .xls file.

• Yes

Relevant data will be deposited and shared in KU Leuven Research Data Repository (RDR), which uses DataCite as metadata standard.

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

Where will the data be stored?

Data will be stored on computers of the researchers involved in the research project. These computers automatically store the data on the OneDrive cloud server.

How will the data be backed up?

Backups of the university's central servers are automated.

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

Standard storage space provided by KU Leuven suffices.

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

Access to the OneDrive cloud server is protected by the KU Leuven authenticator service.

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

No additional costs for data storage and backup are expected.

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...).

Relevant data will be stored on the university's central servers with automatic back-up procedures for at least 10 years, conform the KU Leuven RDM policy.

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

Relevant data will be stored on the university's central servers with automatic back-up procedures for at least 10 years, conform the KU Leuven RDM policy. Physical data will be stored in the laboratories of KU Leuven.

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

No additional costs for data preservation are expected.

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 an Open Access repository

Relevant data accompanying a publications of the research results will be uploaded as supplementary information. Relevant data will be deposited and shared in KU Leuven RDR. Any additional data information can be requested by e-mail.

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

Research data will be publicly available as supplementary information to publications in scientific journals. Any additional data information can be requested by e-mail.

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

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

The relevant data will be made publicly available in the Research Data Repository (RDR) of KU Leuven.

When will the data be made available?

Upon publication of research results.

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

Not applicable.

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.

• Yes

The relevant data will be made available in the Research Data Repository (RDR) of KU Leuven, which uses a DOI number to identify the data.

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

No additional costs for data sharing are expected.

6. Responsibilities

Who will manage data documentation and metadata during the research project?				
Anke Snauwaert				
Who will manage data storage and backup during the research project?				
Anke Snauwaert				
Who will manage data preservation and sharing?				
Anke Snauwaert				
Who will update and implement this DMP?				
Anke Snauwaert				