Zeolite synthesis in a milli-fluidic ultrasonic flow reactor

A Data Management Plan created using DMPonline.be

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Project abstract:

Zeolites are nowadays attractive crystalline porous materials thanks to their wide application range in the chemical industry, as catalysts, adsorbents, ion exchangers, drug carriers. Industrial zeolite synthesis via hydrothermal method still relies on batch reactors. However, poor mass and heat transfer in such systems strongly limit the speed of the process and the synthesis temperatures. A shift towards continuous manufacturing would allow shortening synthesis times, although the presence of a solid phase in the system causes deposition and clogging of the channels. Ultrasound is seen as a valuable tool to overcome such an issue. Moreover, the formation and burst of cavitation bubbles intensifies mixing, improves mass and heat transfer, and forms radicals, which could be exploited in the zeolite synthesis.

In this project, different zeolites synthesis methodologies are developed and optimized in a milli-fluidic ultrasonic flow reactor. Cavitation activity and flow behaviour under sonication are first quantified, to find the optimal synthesis conditions, supported with population balance equation modelling. Subsequently, interzeolite conversion, traditional hydrothermal, seed-aided and OSDA-free syntheses routes are explored to successfully produce zeolites under sonication and in flow.

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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)

The research will generate new data, which will not refer to any identifiable natural person. Microsoft Excel (.xlsx, .csv) data are generated from XRD analysis (original .raw data and .udf intermediate saving), from ICP analysis, from fluorimetry measurements, which are further elaborated in MATLAB (.m). Images are generated from SEM analysis as .tiff files, microscope images as .jpeg, .png files. BET data as .pdf and further exported as .xlsx or .txt file for further elaboration. Temperature recordings are saved as .ghf, .txt, .dat files. Tables, scripts, procedures are generated and saved as .xlsx and .docx files. Graphs are created in MATLAB (.m files, saved as .png) or Origin (.eps, .opj, .png).
Unknown file format for FTIR analysis, RTD measurements and Villermaux-Dushman experiments.

The estimated total data volume for the entire research project is 2 TB.

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.)

During the research: Elena Brozzi; After the research: Prof. Simon Kuhn

1. Storage capacity/repository
    - during the research
    - after the research

Data will be stored during the research on a hard drive, on the work laptop of the researcher and on OneDrive cloud storage. After completion of each WP, as well as after any publication of an article, data will be stored additionally in the university central server.

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)

No

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

None

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DPIA

DPIA

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

- Not applicable

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GDPR

GDPR

Have you registered personal data processing activities for this project?

- Not applicable

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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	*Please choose from the following options:* • Observational • Experimental • Compiled/aggregated data • Simulation data • Software • Other • NA	*Please choose from the following options:* • .por, .xml, .tab, .cvs,.pdf, .txt, .rtf, .dwg, .gml, … • NA	*Please choose from the following options:* • <100MB • <1GB • <100GB • <1TB • <5TB • <10TB • <50TB • >50TB • NA	
Zeolite	Solid material	New	Physical				Every sample <2 g
HTA solution	Product of terephthalic acid dosimetry	New	Physical				Every sample < 20 mL
Iodine solution	Product of Villermaux-Dushman protocol	New	Physical				Every sample < 20 mL
X-Ray Diffraction	Crystallinity patterns for zeolites	New	Digital	Experimental	.raw, .udf, .xslx	< 100 MB	
Scanning Electron Microscopy	SEM pictures for morphology and particle size determination	New	Digital	Experimental	.tiff	< 1 TB	
Temperature control	Recording of the temperature trend over time	New	Digital	Experimental	.txt, .dat, .ghf	< 100 MB	
ICP-OES	Elemental concentration and Si/Al ratio determination	New	Digital	Experimental	.xlsx	< 100 MB	
FTIR	Al distribution and bond stretching observation	New	Digital	Experimental	.csv, .spg	< 100 MB	
N2 physisorption (BET)	Pore size distribution, pore volume and surface area	New	Digital	Experimental	.pdf, .xslx	< 100 MB	
PBM for IZC	Population balance model development for IZC	New	Digital	Simulation data	.m, .png, .txt	< 500 GB	
Manuscripts/presentations	Written texts, notes, visuals	New	Digital	Compiled/aggregated data	.docx, .ppt, .pdf	< 1 GB	
Images	Graphics	New	Digital	Compiled/aggregated data	.psd, .eps, .ai	< 100 GB	
Plots and graphs	Visualization of data, data elaboration	New	Digital	Compiled/aggregated data	.m, .png, .tiff, .opj	< 1 GB	
3D printing	design of parts of the setup	New	Digital	Compiled/aggregated	.stl, .form	< 100 MB	
Photos	Pictures of set up and reactors	New	Digital	Experimental	.png, .jpeg	< 1 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:

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).

- Zeolite: solid material will be stored according to safety standards. Every sample is labelled unambiguously and every experimental campaign is recorded in an electronic list (.docx, .xlsx). Procedures for zeolite synthesis are reported digitally (.docx) and observation are written in a lab notebook, subsequently reported and saved digitally.
- HTA solution: solution vials are stored according to safety standard and protocols. Samples are labelled unambiguously and every experimental campaign is recorded in an electronic list (.docx, .xlsx). Terephthalic acid dosimetry protocols and experimental conditions are reported digitally (.docx) and observation are written in a lab notebook, subsequently reported and saved digitally.
- Iodine solution: solution vials are stored according to safety standard and protocols. Samples are labelled unambiguously and every experimental campaign is recorded in an electronic list (.docx, .xlsx). Villermaux-Dushman protocols and experimental conditions are reported digitally (.docx) and observation are written in a lab notebook, subsequently reported and saved digitally.
- X-Ray Diffraction: Data are received in .raw and named as "name_time_conditions". Standard Operating Procedures (SOP) are followed to carry the analysis. Observations and procedures are reported in a handwritten lab book and subsequently noted digitally (.docx, .xlsx). Data analysis and elaboration will produce .xlsx spreadsheets. After operation, samples are not stored but can be partially recuperated.
- Scanning Electron Microscopy: Pictures are taken according SOPs and saved in .tiff and named "name_time_conditions", as the device settings are displayed on the pictures taken. ImageJ software can be used to analyse the images and produce particle size distributions with the use of MATLAB software (.m, .xlsx). After operation, samples are not stored.
- Temperature control: SE520 software is used to record temperature over time. Data are saved in .txt, .dat or .ghf. Operating conditions are handwritten in a lab notebook and subsequently reported electronically (.docx, .xlsx). Data are elaborated with MATLAB software.
- ICP-OES: Samples are prepared according to SOPs and named "name_time_conditions". Observations and procedures are reported in a handwritten lab book and subsequently noted digitally (.docx, .xlsx). Data are received in .csv, .xlsx format. After operation, samples are not stored.
- FTIR: Samples are prepared according to SOPs and named "name_time_conditions". Observations and procedures are reported in a handwritten lab book and subsequently noted digitally (.docx, .xlsx). After operation, samples are not stored but can be partially recuperated.
- N2 physisorption: Samples are prepared according to SOPs and named "name_time_conditions". Observations and procedures are reported in a handwritten lab book and subsequently noted digitally (.docx, .xlsx). After operation, samples are not stored. .pdf data are produced and converted to .xlsx files.
- PBM for IZC: Simulations are carried out via MATLAB software (.m). Readme files (.txt) are produced to record steps and procedures and stored on a private GitHub profile.
- Manuscripts: Manuscripts of performed research are compiled and saved in .docx, .pdf or .tex format.
- Presentations: Dissemination of the information is produced and saved in .ppt and .pdf.
- Images: Images are created using Adobe Photoshop, Illustrator softwares. They are originally stored in .psd and .ai format, subsequently exported to .eps, .tiff, .png according to necessity.
- Plots and graphs: Plots and graphs are produced from .xlsx data by using MATLAB and Origin softwares (.m, .opj). The elaborated data are then saved in .png format.
- 3D printing: SolidEdge and Fusion360 softwares are used to produce .stl files, which are subsequently used for 3D printing of such models. 3D printed models are physically stored.
- Photos: Relevant photos of the set-up, the reactors are stored in .jpeg, .tiff format.

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

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

Where will the data be stored?

All data will be stored in a shared cloud (OneDrive), as well as on the work laptop of the researcher and on external hard drive. After completion of WPs, data will be additionally stored in the KUL service servers.

How will the data be backed up?

Data are backed up on the cloud (OneDrive) immediately. The system automatically indicates the update state (green, blue or red). In case of a nonsync
with the online (red), action is taken via the online (browser) version of the tool to ensure syncing. Data are further backed up regularly on an external hard drive. After completion of WPs, data will be additionally backed up in the KUL service servers.

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

Data storage should not exceed 2 TB.

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

The accesses to the OneDrive and sharepoint are only for researchers with permission. All users need to use a two-factors Authenticator (2FA app used at KUL).
Furthermore, a log-out is always performed when leaving LAB PCs (where data is generated) to prevent modification of parameters by unauthorized persons.

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

The expected costs for data storage and back up during the project will be 5000€.
These costs will be covered by Prof. Simon Kuhn.

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 retained for at least 5 years and we will not deviate from that.

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

All data will be retained for the expected 5 year period after the end of the project. The data will be stored on the university's central servers (with automatic back-up procedures), conforming with KUL RDM policy.

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

The complete datasets will be hosted on the servers of KU Leuven. The expected costs of data storage and preservation will be approximately 5000€. This cost will be covered by Prof. Simon Kuhn.

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
- Yes, in a restricted access repository (after approval, institutional access only, …)

Relevant data for publication will be made available in Open Access repository. Full datasets can be made available upon request.

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

Not applicable

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.

Data used for publication will be made available via Open Access repositories. Further data can be made available upon request via email to the researcher and/or to the responsible of the data after research.

When will the data be made available?

Data will be made available upon publications of the research results.

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

There are no data that require a usage license.

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 expected cost for data sharing is 0€. Free data sharing tools (e.g. WeTransfer) can be used for data sharing. In the unlikely event there will be costs, these costs will be covered by Prof. Simon Kuhn.

6. Responsibilities

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

Elena Brozzi

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

Elena Brozzi

Who will manage data preservation and sharing?

Prof. Simon Kuhn

Who will update and implement this DMP?

Elena Brozzi. Prof. Simon Kuhn bears the end responsibility of updating and implementing this DMP in the long term.