Photooxidation of antibiotics in multiphase flow in a microreactor by using visible-light active red mud-based geopolymers

A Data Management Plan created using DMPonline.be

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Project abstract:

Removing antibiotics from wastewater requires further attention because of a continuously increased pollution level. One of the prominent ways to remove antibiotics is through advanced oxidation processes that are primarily performed in batch reactors. Batch reactors suffer from poor mass and photon transfer, which is especially problematic for photocatalytic oxidation processes as this strongly limits the efficacy of the process. Transitioning to continuous processes in microreactors will overcome these limitations and provide a fundamental framework for the degradation kinetics of antibiotics.

This project introduces visible-light active and magnetic geopolymers from industrial waste for degrading antibiotics in a three-phase flow in a continuous photo-microreactor. The magnetic separability and photocatalytic activity of waste red mud-based geopolymers are first provided by using commercial chemicals. They are then used to identify the optimum reaction conditions and characterize the flow hydrodynamics. Subsequently, their application to different antibiotics and real wastewater is studied, and corresponding kinetic analyses are made. Lastly, their entirely red mud-based counterpart is synthesized to determine its performance for the photodegradation of antibiotics. By combining the merits of microfluidics and the photocatalytic oxidation processes, this project provides a sustainable direction for using waste based materials in multiphase systems for wastewater treatment.

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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:	*Please choose from the following options:*	*Please choose from the following options:*	*Please choose from the following options:*	*Please choose from the following options:*	
		Generate new data	Digital	Observational	.por, .xml, .tab, .cvs,.pdf, .txt, .rtf, .dwg, .gml, …	<100MB	
		Reuse existing data	Physical	Experimental	NA	<1GB	
				Compiled/aggregated data		<100GB	
				Simulation data		<1TB	
				Software		<5TB	
				Other		<10TB	
				NA		<50TB	
						>50TB	
						NA	
Photocatalyst	Solid powder material	New	Physical				Every sample <2 g
Red mud-based geopolymer	Solid powder material	New	Physical				Every sample <2 g
Photocatalyst incorporated red mud-based geopolymer	Solid powder material	New	Physical				Every sample <3 g
X-Ray Diffraction	Crystallinity patterns for zeolites	New	Digital	Experimental	.raw, .udf, .xslx	< 200 MB	
Scanning Electron Microscopy	SEM pictures for morphology and particle size determination	New	Digital	Experimental	.tiff	< 1 TB	
Photoluminescence spectroscopy	To determine the recombination of electron-hole and to study charge transfer properties	New	Digital	Experimental	.csv	< 100 MB	

Diffuse reflectance spectroscopy	Optical absorption and band-gap of the materials	New	Digital	Experimental	.csv	< 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	
UV-Vis spectroscopy	To determine the absorption spectrum of antibiotic solutions	New	Digital	Experimental	.txt	< 100 MB	
Electron spin resonance spectroscopy	To determine the oxygen vacancies	New	Digital	Experimental	.txt, .csv	< 100 MB	
X-ray photoelectron spectroscopy	Oxidation state of the elements present on the surface of the material	New	Digital	Experimental	.vgx	< 1 GB	
Manuscripts/presentations	Written texts, notes, visuals	New	Digital	Compiled/aggregated data	.docx, .ppt, .pdf	< 5 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	< 2 GB	
3D printing	Design of parts of the photo-reactor	New	Digital	Compiled/aggregated data	.stl, .form	< 100 MB	
Photos	Pictures of set up and reactors	New	Digital	Experimental	.png, .jpeg	< 1 GB	
Videos of the experimental setup	Videos of set up and reactors	New	Digital	Experimental	.mp4	< 2 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).

- Photocatalyst: Catalysts will be stored following safety standards. Every sample is labeled unambiguously and every experimental campaign is recorded in an electronic list (i.e. an electronic lab notebook in .xls and OneNote). The methodology and protocol for handling the catalysts will be taken from reported procedures as much as possible and/or described in detail in a lab book.

- Red mud-based geopolymer: Geopolymers will be stored by safety standards. Every sample is labeled unambiguously and every experimental campaign is recorded in an electronic list (i.e. an electronic lab notebook in .xls and OneNote). The methodology and protocol for handling the catalysts will be taken from reported procedures as much as possible and/or described in detail in a lab book.

- Photocatalyst-incorporated red mud-based geopolymer: Photocatalyst-incorporated red mud-based geopolymer will be stored following safety standards. Every sample is labeled unambiguously and every experimental campaign is recorded in an electronic list (i.e. an electronic lab notebook in .xls and OneNote). The methodology and protocol for handling the catalysts will be taken from reported procedures as much as possible and/or described in detail in a lab book.
- X-Ray Diffraction: Data are received in .raw and named "name_time_conditions". Standard Operating Procedures (SOP) are followed to carry out 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 to 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 analyze the images and produce particle size distributions with the use of MATLAB software (.m, .xlsx). After operation, samples are not stored.
- Photoluminescence spectroscopy: Data received in .csv format are named "name_time_conditions". After operation, samples are not stored.
- Diffuse reflectance spectroscopy: Data are received in .csv and named "name_time_synthesisconditions". Standard Operating Procedures (SOP) are followed to carry out the analysis. Data analysis and elaboration will produce .xlsx spreadsheets. After operation, samples are stored.
- 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 and .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 (BET): 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.
- UV-Vis spectroscopy: Data received in .txt format are named "name_time_conditions". After operation, samples are not stored.

- Electron spin resonance spectroscopy: Data received in .txt and .csv format are named "name_time_conditions". After operation, samples are not stored.
- X-ray photoelectron spectroscopy: Data received in .vgx format are named "name_time_conditions". After operation, samples are not

stored.

- Manuscripts: Manuscripts of performed research are compiled and saved in .docx, .pdf or .txt format.
- Presentations: Presentations of performed research are compiled and saved in .ppt or.pdf format.
- Images: Images are created using Adobe Photoshop, and Illustrator software. They are originally stored in .psd and .ai format and subsequently exported to .eps, .tiff, and .png according to necessity.
- Plots and graphs: Plots and graphs are produced from .xlsx data by using MATLAB and Origin software (.m, .opj). The elaborated data are then saved in .png format.
- 3D printing: SolidEdge and Fusion360 software 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, and the reactors are stored in .jpeg, .tiff format.
- Videos of the experimental setup: Videos of the experimental setup and reactors will be saved in .mp4 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 an 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 non-sync 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

Maximum 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 OneDrive and SharePoint are only for researchers with permission. All users need to use a two-factor 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 e-mail to the researcher and/or to the responsible for 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?

Kardelen Kaya Özkiper

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

Kardelen Kaya Özkiper

Who will manage data preservation and sharing?

Prof. Simon Kuhn

Who will update and implement this DMP?

Kardelen Kaya Özkiper and Prof. Simon Kuhn bears the end responsibility of updating and implementing this DMP in the long term.