Lab test platform for electrification and sustainable continuous chemical processes

A Data Management Plan created using DMPonline.be

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Project abstract:

The International Energy Agency's Net Zero by 2050 report identifies the industry as the second-largest global source of CO2 emissions within the energy sector, with the chemicals, steel, and cement industries responsible for 70% of these emissions. Furthermore, the European Union has incorporated this commitment to climate action through the European Climate Law, effective since July 29, 2021. This legislation mandates achieving climate neutrality by 2050 and reducing net greenhouse gas emissions by at least 55% by 2030. One of the technological pathways outlined in the ERA industrial technology roadmap to achieve this objective is through electrification, using electricity generated from sustainable sources as the primary energy source. This challenges current chemical industry norms. Addressing this, the HITEC center is established (https://hitec-center.eu/) with a distinctive portfolio that enables the aforementioned transition by offering solutions for batch-to-flow conversion, electricity-based activation (such as through light, sound, and electrochemical processes), and electricity-based stimulation of fluid flow to improve mixing. However, our technologies are currently at a TRL of 3-4, validated in laboratory settings. The aim is to raise them to TRL 5-6, where they are validated and demonstrated in an industrially-relevant setting. This project aims to bridge the gap by: (1) Expanding of the range of operating conditions and catering to the specific needs of processes by enhancing realization capabilities using CNC technology in the development phase; (2) Development of complete system designs with online analysis capability and definition of control systems and philosophies to facilitate faster testing, data collection, and evaluation in the design & maturation phases; (3) Demonstration of better readiness for handling various process environments with industrial-relevant case studies

Last modified: 13-05-2024

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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: **N**(ew data) or **E**(xisting data)*	Indicate: **D**(igital) or **P**(hysical)	Indicate: **A**udiovisual **I**mages **S**ound **N**umerical **T**extual **M**odel **SO**ftware Other (specify)		Indicate: <1GB <100GB <1TB <5TB >5TB NA	
p-nitrophenyl acetate solution	Aqueous solution 0.05M max	N	P				Every sample (1.5 ml)
Degraded phenol solution	Aqueous solution 100 mg/l max	N	P				Every sample (1.5 ml)
O-Aminobenzoic acids form III	Solid Crystals	N	P				Every sample 10 g.
FTIR	To identify newly formed bonds in the liquid/solid phases	N	D	N,T	.csv, .spg	< 1 GB	
UV-Vis spectroscopy	To determine the absorption spectrum of phenol solution	N	D	N,T	.txt	< 1 GB	
X-Ray Diffraction	Identify the morphology of the crystals formed	N	D	N,T	raw, .udf, .xslx	< 1 GB	
3D printing	Design of the reactor parts	N	D	M	.stl, .form	< 1 GB	
mechanical manufacturing	Design of reactor parts with CNC in Autocad	N	D	M	.dwg	< 1 GB	
Hi-speed camera images	Flow behaviour in continuous reactor.	N	D	I, A	.raww, .mp4,.avi, .png, .jpeg	< 5 TB	
Images	Graphics, P&IDS	N	D	I	.png, .jpeg, .dwg, .pdf	<1 GB	
Videos of the experimental setup	videos of physical experimental observations and workings	N	D	A	.raww, .mp4,.avi	< 100 GB	
Notes	Daily lab observations	N	D	N,T	.one, .xlxs, .docx, .pdf	< 1 GB	
plots and graphs	Visualization of data, data elaboration	N	D	N, T, I	.xlxs, .docx, .pdf, .png, .jpeg	< 1 GB	
Manuscripts/ presentations	Written texts, notes, visuals	N	D	N, T, I	.xlxs, .docx, .pdf, .png, .jpeg, .ppt	< 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:

Zhang, S., Junkers, T., & Kuhn, S. (2022). Continuous-flow self-supported seATRP using a sonicated microreactor. Chemical Science, 13(42), 12326–12331. https://doi.org/10.1039/d2sc03608h

Hussain, M. N., Jordens, J., John, J. J., Braeken, L., & Van Gerven, T. (2019). Enhancing pharmaceutical crystallization in a flow crystallizer with ultrasound: Anti-solvent crystallization. Ultrasonics Sonochemistry, 59(March). https://doi.org/10.1016/j.ultsonch.2019.104743

John, J. J., Kuhn, S., Braeken, L., & Gerven, T. Van. (2017). Temperature controlled interval contact design for ultrasound assisted liquid-liquid extraction. Chemical Engineering Research and Design, 125, 146–155. https://doi.org/10.1016/j.cherd.2017.06.025

John, J. J., Kuhn, S., Braeken, L., & Van Gerven, T. (2017). Ultrasound assisted liquid-liquid extraction with a novel interval-contact reactor. Chemical Engineering and Processing: Process Intensification, 113, 35–41. https://doi.org/10.1016/j.cep.2016.09.008

Kaya-Özkiper, K., Mc Carogher, K., Roibu, A., & Kuhn, S. (2023). Photo-Oxidation in Three-Phase Flow with Continuous Photosensitizer Recycling. ACS Sustainable Chemistry and Engineering, 11(26), 9761–9772. https://doi.org/10.1021/acssuschemeng.3c01869

Mc Carogher, K., Dong, Z., Stephens, D. S., Leblebici, M. E., Mettin, R., & Kuhn, S. (2021). Acoustic resonance and atomization for gas-liquid systems in microreactors. Ultrasonics Sonochemistry, 75, 105611. https://doi.org/10.1016/j.ultsonch.2021.105611

van Stee, J., Hermans, G., John, J. J., Binnemans, K., & Van Gerven, T. (2024). Cobalt/nickel purification by solvent extraction with ionic liquids in millifluidic reactors: From single-channel to numbered-up configuration with solvent recycle. Chemical Engineering Journal, 479, 147234. https://doi.org/10.1016/J.CEJ.2023.147234

van Stee, J., Keppens, F., John, J. J., Binnemans, K., & Van Gerven, T. (2023). Can 3D printing solve the numbering-up challenge of microfluidic reactors? Chemical Engineering Research and Design, 197, 127–135. https://doi.org/10.1016/J.CHERD.2023.07.022

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

3D printing	Potential designs for patent / tech transfer spinoff
mechanical manufacturing	Potential designs for patent / tech transfer spinoff
Hi-speed camera images	Validation of effects for patent / tech transfer spinoff
Images	Quantified novel effects for patent / tech transfer spinoff
Videos of the experimental setup	Validation of effects for patent / tech transfer spinoff
Notes	Quantified novel effects for patent / tech transfer spinoff
plots and graphs	Quantified novel effects for patent / tech transfer spinoff
Manuscripts/ presentations	complete description of novel effects for patent / tech transfer spinoff

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.

- 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

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).

- **p-nitrophenyl acetate solution:** Vials containing the solution are stored in the lab according to safety standards. Every sample will be labelled unambiguously (“name_time_conditions”) and will be recorded in a lab notebook. Subsequently, the sample name (combined with the corresponding conditions and observations) is added and saved into an electronic list (.docx, .xlsx), which also contains a more detailed description of the followed experimental procedure.
- **Degraded phenol solution:** Vials containing the solution are stored in the lab according to safety standards. Every sample will be labelled unambiguously (“name_time_conditions”) and will be recorded in a lab notebook. Subsequently, the sample name (combined with the corresponding conditions and observations) is added and saved into an electronic list (.docx, .xlsx), which also contains a more detailed description of the followed experimental procedure.
- ***O*-Aminobenzoic acids form III:** Created crystalline material will be stored in the lab according to safety standards and protocols. Every sample will be labelled unambiguously (“name_time_conditions”) and will be recorded in a lab notebook. Subsequently, the sample name (combined with the corresponding conditions and observations) is added and saved into an electronic list (.docx, .xlsx), which also contains a more detailed description of the followed experimental procedure.
- **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.
- **UV-Vis spectroscopy:** Data received in .txt format are name "name_time_conditions". After operation, samples are not stored.
- **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.
- **3D printing:** 3D models for setup construction are design in Solid Edge (.par) and saved digitally. After exporting the 3D model into an .stl file, the physical part is made by 3D printing. Both the .stl files as the physical part will be stored (either digitally or inside a setup).
- **Mechanical manufacturing:** 3D models are design in autocad (.dwg) and converted to a step file (.stp) for the CNC machine. After exporting the physical part is made by the CNC. Both the .stp files as well as the physical part will be stored (either digitally or inside a setup).
- **Hi-speed camera images:** Pictures are taken according to SOPs and saved in .raww, .png, .jpeg or as short movies in .mp4 or ,avi and named "name_time_conditions", as the device settings are displayed on the pictures taken. Image J software can be used to analyze the images and produce particle size distributions with the use of MATLAB software (.m, .xlsx)
- Images: Images are created using Adobe Photoshop, or inkscape. They are originally stored in .psd and .svg format and subsequently exported to .tiff, .pdf and .png according to necessity.
- **Videos of the experimental setup:** Videos of the experimental setup and reactors will be saved in .mp4 or .avi format
- **Notes:** The physical lab notebook is used for setup design (sketches) and for writing down of observations a digital notebbook OneNote will be used. When not used in the lab, the physical notebook will be stored in a locked drawer in the office. The digital note book will be made available to the required personal by giving the said person access via teams. The digital notebook will be stored as .one format.
- **plots and graphs** : Data from experiments or simulations are provided as .txt files that can be plotted using excel or origin software. the files will be stroed digitally as .xlxs or .opj files. The output can be obtained in the file type required. like.png, .pdf, .tiff depending on the final application of the plot/graph.
- **Manuscripts/ presentations:** Manuscripts or presentations of performed research are compiled and saved in .docx, .pdf, .ppt or .txt format.

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.

- No

Data Storage & Back-up during the Research Project

Where will the data be stored?

- OneDrive (KU Leuven)
- Large Volume Storage
- Personal network drive (I-drive)

All data will be stored on the work laptop of the researcher, on an external hard drive and in a shared cloud (OneDrive). After completion of (sub)WPs, the data will be additionally stored on the KUL service servers or the TVG - NAS network drive.

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?

Only authorized researchers have access to the OneDrive account: all users need to use a two-factor authentication to log in (MFA app from KUL). On lab computers, a log-out is always performed to prevent modification by unauthorized people. Hard drives and physical lab notebooks are stored in a closed drawer in the office.

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. Tom Van Gerven and Prof. Simon Kuhn

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)?

- Large Volume Storage (longterm for large volumes)

The complete datasets will be hosted on the servers of KU Leuven and stored in large volume storage network drive.

What are the expected costs for data preservation during the expected retention period? 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. Tom Van Gerven and Prof. Simon Kuhn.

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

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.

Prof. Tom Van Gerven and Prof. Simon Kuhn will be able to access the data and upon their evaluation of relevance, the data will made available.

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.

- No

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)

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.

- Other (specify below)

To be specified later.

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.

- No

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

NA

Responsibilities

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

Professors (Tom Van Gerven & Simon Kuhn)
Research Expert (Jinu Joseph John)

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

internal storage is used via ICTS KU Leuven.

Who will manage data preservation and sharing?

Professors (Tom Van Gerven & Simon Kuhn)

Who will update and implement this DMP?

Professors (Tom Van Gerven & Simon Kuhn)
Research Expert (Jinu Joseph John)