Plan Overview

A Data Management Plan created using DMPonline.be

Title: Catalytic conversion of ethylene and CO2 in supercritical conditions

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Funder: Fonds voor Wetenschappelijk Onderzoek - Research Foundation Flanders (FWO)

Template: FWO DMP (Flemish Standard DMP)

Project abstract:

Aromatics such as benzene, toluene, and xylenes (BTX), are crucial chemical building blocks for plastics and fine chemicals. Currently, BTX production relies heavily on by-products from fossil naphtha cracking. An underexplored avenue involves synthesizing BTX directly from ethylene (accessible from bio-ethanol or methanol-to-olefins) through heterogeneous catalysis. However, rapid deactivation due to coking poses a significant and unresolved challenge. Exploring catalytic reactions in supercritical conditions (Sc) emerges as a promising yet largely untapped strategy. This approach
enhances reactants and products solubilities and diffusivity within the catalyst, leading to unexpected increases in product yields. Notably, it also offers a potential solution to overcoming deactivation by carbon species deposition. This project aims to develop a catalytic system for supercritical ethylene aromatization using zeolite-based catalysts. In particular, Zn and Ga based catalysts will be synthesized to achieve the best selectivity to BTX at low temperature (<<573 K) and moderate (but sc) pressures (50-100 bar). To ensure stable performance over time, also supercritical CO2 will be explored as a co-solvent for catalyst regeneration and potentially to prevent deactivation. Additionally, this project seeks to break new ground by delivering proof of concept of combining supercritical CO2 as a reactant with ethylene for the direct synthesis of acrylic acid under supercritical conditions.

ID: 212923

Start date: 01-10-2024

End date: 30-09-2027

Last modified: 18-02-2025

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FWO DMP (Flemish Standard DMP)

1. Research Data Summary

				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, .csv,.pdf, .txt, .rtf, .dwg, .gml, … • NA	*Please choose from the following options:* • <100MB • <1GB • <100GB • <1TB • <5TB • <10TB • <50TB • >50TB • NA	
Catalyst	Solid materials	new	Physical	/	/	/	>200g
Microscopy	Microscopy	new	Digital	Experimental	.jpeg or .tif	<100MB	/
Spectroscopy	FTIR, TPD, TGA, NMR...	new	Digital	Experimental	.spg or .csv	<100GB	/
Diffraction patterns	difracction patterns (XRD)	new	Digital	Experimental	.raw	<100MB	/
Manuscripts/presentations	Textual data	new	Digital	Experimental	.docx, .pptx, .pdf	<100MB	/
Plotting worksheets	worksheets	new	Digital	Experimental	.csv, .xls	<100MB	/
chromatograms	chromatograms	new	Digital	Experimental	.xls	<100MB	/
Python codes	programming codes for calculations	new	Digital	Experimental	.py	<100MB	/

no reuse of existing data

- No

- No

- Yes

IP generation is possible when unexpected, original materials or processes are created. When suited: the steps for IP generation will be evaluated and checked.
IP restrictions: waiting for publication or public availability of key observations until after first patent deposition + few months

- No

- No

2. Documentation and Metadata

- Catalysts will be stored in accordance to safety standards. Labels will be added with inambigous conection to an electronic list (i.e. an electronic lab notebook in .xls).
- The methodology and protocol during handling of the catalysts will be take from reported procedures as much as possible and/or described in details in a lab book.
- Microscopy images (.jpeg) will be noted as: sample code_image type_bit-depth_microscope settings_date. A standard operation procedure (SOP) is used if possible. The methodology and
protocol will be described in details in the lab book.
- X-ray diffraction patterns (.xls) will be noted as: sample code_scans settings_XRD parameters_date. A standard operation procedure (SOP) is used. The protocol of the sample preparation will be described in the lab book.
- GC data (.CSV) will be noted as: sample code_reaction conditions_GC method parameters_date. A standard operation procedure (SOP) is used if possible and the protocol and reactions conditions will be described in the lab book.
- FT-IR spectra (.spg) will be noted as: sample code_conditions_machine settings_date. A standard operation procedure (SOP) is used if possible. The analysis method and the sample preparation will be described in the lab book.
- NMR data (.zip folder) will be noted as: sample code_solvent_reaction conditions_NMR parameters_date. A standard operation procedure (SOP) is used if possible. The protocol of the sample preparation will be described in the lab book.
- Manuscripts/presentations - content related to dissemination (.docx, .pptx, .pdf), and will be noted as:year_title_main participant (contributors)
- Worksheets for basic calculations and making visualizations/plots (.xls)
- Python files will be noted as: test description.py (.py)

- No

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

All data during this project will be stored on the shared cloud (OneDrive). Access is possible on both the PC or online.

The backup of the data during this project will be automatically done on the shared cloud (OneDrive). 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.
Some folders are shared. If I am the folder owner with other people able to edit/remove data, I take trimestral backups. For extra security, the publishable data will be collected in a separate
folder and also back-uped on an individual external device.

- Yes

Maximum data storage should not exceed 500 GB.

The accesses to the OneDrive and sharepoint are only for researchers with permission. All users need to use an 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.

With the project funding, an external offline hard drive will be purchased for offline storage

4. Data preservation after the end of the research project

Due to the estimated small size of the data, all the extracted data can be retained for the expected 5 year period after the end of the project.

After the project, key data (especially the 'publishable data' folder) will be stored on Box with backup on an external hard drive (1TB) with the promotor.

The estimated cost of the external hard drive (1TB) is around 50-100euro.

5. Data sharing and reuse

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

The valuable data and the ones related to accepted (or pending) publications will be available. Ideady, it is published in Open Access.

N.A.

- No

In publications or more detailed things upon request by mail.
Reasonable requests for data can be done by email from the PI of the project, data can be sent by email or via wetransfer.

Upon publication of the research results.

No data under licenses.

- No

Requested data will be free of charge, free data transfer links will be used (or emails if few Mbs).

6. Responsibilities

Giovanni Pampararo

Giovanni Pampararo (mainly) and prof. Michiel Dusselier (PI)

prof. Michiel Dusselier (PI)

Giovanni Pampararo. The PI bears the end responsibility of updating & implementing this DMP.