DMP title

Project Name - Dual catalysis approach for the carboxylation of aliphatic olefins using CO_2 as the carbon source (2CCO$_2$, 2 catalysts for CO_2)

Grant Title HBC.2021.0588

Principal Investigator / Researcher Dirk De Vos

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Description 2CCO$_2$ aims at forming carboxylic acids or carboxylate esters **directly from CO$_2$ and olefins**, using a minimal amount of hydrogen, viz. 1 molecule of H_2 per molecule of CO_2. To this aim, the Reverse Water Gas Shift reaction (RWGSR) is coupled *in situ* to various types of olefin carbonylation, in the same conditions of temperature and pressure.

This approach allows to **shift the equilibrium of the RWGSR** (which is limited to a few % by thermodynamics at temperatures of 150-200°C) to the CO-side, since the CO is continuously consumed in the ensuing carbonylation reaction. The crucial innovation is to physically separate the homogeneous catalyst for alkoxycarbonylation and the solid catalyst for RWGSR, even if they are in the same reactor. Practically this is achieved by entrapping the RWGSR catalytic function in a shape-selective zeolite, while the homogeneous catalyst operates in the surrounding liquid. The objectives aim at first developing catalysts for the RWGSR (Obj. 1) and the carbonylation (Obj. 2), striving for shape-selectivity of the zeolite and mutual compatibility of both catalysts / reactions. The concept of equilibrium shifting is then tested by bringing both catalysts together in one pot (Obj. 3); finally the adsorption and diffusion phenomena in this 3-phase system are studied by experiment and modelling (Obj. 4), in order to maximize compatibility and productivity of both reactions

Institution KU Leuven

1. General Information
Name applicant

Dirk De Vos

Project Number & Title

HBC.2021.0588 Dual catalysis approach for the carboxylation of aliphatic olefins using CO_2 as the carbon source (2CCO$_2$, 2 catalysts for CO_2)

Affiliation

KU Leuven

2. Data description
Will you generate/collect new data and/or make use of existing data?

Generate new data

Describe in detail the origin, type and format of the data (per dataset) and its (estimated) volume. This may be easiest in a table (see example) or as a data flow andper WP or objective of the project. If you reuse existing data, specify the source of these data. Distinguish data types (the kind of content) from data formats (the technical format).

We will perform catalytic reactions, prepare catalysts and collect and interpret reaction data. Such procedures will result in raw data files containing chromatographic data (GC-FID, GC-MS, LC, LCMS, FTIR) and material characterization data (XRD, XAS data, physisorption and chemisorption data or spectroscopic analysis via FTIR, NMR etc.). These will be processed in excel files, summaries and presentations, finally culminating in manuscripts and/or patents. The combined virtual volume of these datasets will be limited (< 20 GB), and willconsist mostly of data files containing GC chromatograms (up to 5 GB).

Examples:

Type of data	Format	Volume	How created
X-ray diffractaction patterns	.xrdml	20 kB	XRD spectroscopy of synthesized catalysts
XAS (EXAFS, XANES)	/	100 kB	Synchrotron experiments
GC chromatograms	.gcd	< 2 MB	GC analysis of worked-up reaction samples
NMR spectra	/	256 kB	NMR spectroscopy of synthesized products
FTIR-data	calcmet.spectrum	< 1 MB	FTIR analysis of headspace

3. Legal and ethical issues

Will you use personal data? If so, shortly describe the kind of personal data you willuse. Add the reference to your file in KU Leuven's Register of Data Processing for Research and Public Service Purposes (PRET application). Be aware that registeringthe fact that you process personal data is a legal obligation.

No•

Privacy Registry Reference:

Short description of the kind of personal data that will be used:

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, add the reference to the formalapproval by the relevant ethical review committee(s)

No•

Does your work possibly result in research data with potential for tech transfer and valorisation? Will IP restrictions be claimed for the data you created? If so, for whatdata and which restrictions will be asserted?

Yes•

The methods and reactor configurations developed in this project have potential for valorization,which will be subjected for discussion during the project. Patents will be submitted, transferred and valorized with the assistance of the intellectual property unit of KU Leuven Research & Development (LRD).

Do existing 3rd party agreements restrict dissemination or exploitation of the datayou (re)use? If so, to what data do they relate and what restrictions are in place?

No•

4. Documentation and metadata

What documentation will be provided to enable reuse of the data collected/generatedin this project?

Details to reproduce reaction procedures are described in lab notebooks of the coworkers. Upon presentation or publication of data, procedures are described in sufficient detail to enable a reproduction of the generated results for an experienced user. ReadMe-files or recording methods for advanced characterization are stored in parallel with generated data.

Will a metadata standard be used? If so, describe in detail which standard will beused. If no, state in detail which metadata will be created to make the data easy/easier to find and reuse.

No•

Although no metadata standard is available for the advanced characterization in this project, most techniques store a non-standardized ReadMe-file containing recording parameters and file information in parallel with recorded datasets. Alternatively, some datasets contain metadata headers on recording parameters (e.g. XRD diffractograms, XAS spectra). The data will be stored and named in a consistent manner with unambiguous identifiers. Descriptions of experiments and materials are kept in physical lab notes for each identifier. The data will be processed and summarized in a comprehensive excel worksheet with references to the identifiers. The resulting summaries will culminate in presentations, and finally in manuscripts and/or patents.

5. Data storage and backup during the project
Where will the data be stored?

Physical hand-notes of procedures and initial observations are kept in lab books. Digital data, with unambiguous identifiers for reactions and materials, are kept in cloud storage from 'Box'.KU Leuven offers an Enterprise Box account 3, which offers an easy and secure storage space ofup to 100 GB for each user.

How is backup of the data provided?

By using the cloud storage of OneDrive, digital data will be stored in parallel on the cloud and on the personal computer of the applicant, guaranteeing back-up for this data. Most raw data is also stored and frequently backed up off-line on external hard drives.

Is there currently sufficient storage & backup capacity during the project? If yes, specify concisely. If no or insufficient storage or backup capacities are available thenexplain how this will be taken care of.

Yes•

The cloud storage provides a storage space up to 100 Gb for each user, while the project isexpected to generate less than 10 GB.

What are the expected costs for data storage and back up during the project? Howwill these costs be covered?

Data storage costs on Box are included in an internal service contract with the KU Leuven ITsupport service (SET-IT). No additional costs are expected for the storage of data. In case additional costs do arise, they will be covered by the project budget or reserve funds.

Data security: how will you ensure that the data are securely stored and not accessedor modified by unauthorized persons?

The data will be stored in the university's secure environment for private data. An Enterprise Boxaccount 3 for cloud storage ensures a secure environment.

6. Data preservation after the project
Which data will be retained for the expected 5 year period after the end of the project? In case only a selection of the data can/will be preserved, clearly state thereasons for this (legal or contractual restrictions, physical preservation issues, ...).

All data will be retained for the expected 5 year period after the end of the project.

Where will the data be archived (= stored for the longer term)?

Upon termination of the contract, the data will be transferred and stored on an external harddrive (Samsung Portable SSD T5 1 TB), managed by Annelies Van Vlasselaer.

What are the expected costs for data preservation during the retention period of 5years? How will the costs be covered?

The high capacity of the available external hard drive (1 TB) enables the preservation of data from multiple terminated or finished projects. Currently, an average of 15 GB is used for the finished projects of each user, which allows to divide its cost over approximately 60 users. Giventhe cost of the available hard drive of 120 EUR, the expected costs are negligible. The involved IT-expenses are included in the project's consumable expenses or covered by reserve funds.

7. Data sharing and reuse

Are there any factors restricting or preventing the sharing of (some of) the data (e.g. as defined in an agreement with a 3rd party, legal restrictions)?

No•

Which data will be made available after the end of the project?

Upon publication of the research results, the full datasets will be made available upon reasonablerequest

Where/how will the data be made available for reuse?

Up•n request by mail

When will the data be made available?

Up•n publication of the research results

Who will be able to access the data and under what conditions?

Only uses for research purposes will be allowed and commercial reuse will be excluded.

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

No additional costs are expected as the data can be shared via online platforms (e.g. WeTransfer) or the already budgeted storage cloud from Box. If additional costs would occur theywill be covered from reserve funds.

8. Responsibilities

Who will be responsible for data documentation & metadata?

The applicant (Dirk De Vos).

Who will be responsible for data storage & back up during the project?

The applicant (Dirk De Vos) and Annelies Van Vlasselaer.

Who will be responsible for ensuring data preservation and reuse ?

The supervisor (Dirk De Vos) and Annelies Van Vlasselaer.

Who bears the end responsibility for updating & implementing this DMP?

The applicant (Dirk De Vos) bears the end responsibility ofupdating & implementing this DMP.