

MY PLAN (FWO DMP)

DMP TITLE

ADMIN DETAILS

Project Name: My plan (FWO DMP) - RADIANT

Grant Title: G0A1B24N

Principal Investigator / Researcher: Rob Ameloot

Project Data Contact: rob.ameloot@kuleuven.be

Description: Adsorptive separations by nanoporous materials are major industrial processes. The industrial importance of solid adsorbents is only expected to grow due to the increased focus on carbon dioxide capture technology and energy-efficient separations. To evaluate the performance of an adsorbent and design a separation process, the adsorption thermodynamics and kinetics must be known. Due to the presence of multiple adsorbates in any separation, multicomponent experiments are critical for any industrial process optimization. However, measuring multicomponent adsorption is complex and time-consuming. Measurements of adsorption kinetics are even more challenging. Hence, multicomponent diffusion measurements are rare because of the limitations of the available measurement methods.

By bridging adsorption/diffusion studies and microfabrication, the RADIANT project will develop a new methodology to overcome the challenges related to measuring multicomponent isotherms and diffusivities. Via a novel approach to realize out-of-equilibrium conditions combined with mass spectrometry, the behavior of fast-diffusing molecules will be fully evaluated, even in small adsorbent particles and in both single- and multicomponent scenarios. This methodology will enable the rapid evaluation and selection of adsorbents for separation processes.

Institution: KU Leuven

1. GENERAL INFORMATION

Name applicant

Rob Ameloot

FWO Project Number & Title

Rapid Assessment of Multicomponent Diffusion and Adsorption in Nanoporous Materials (RADIANT)
G0A1B24N

Affiliation

- KU Leuven

2. DATA DESCRIPTION

Will you generate/collect new data and/or make use of existing data?

- Generate new data

Describe the origin, type and format of the data (per dataset) and its (estimated) volume, ideally per objective or WP of the project. You might consider using the table in the guidance.

The expected data volume generated within RADIANT is 1-2 Gb per month.

Objective 1: Rapidly measure multicomponent isotherms

Data related to this objective are mostly the characterization of the prepared samples, including different types of microscopy and spectroscopy. The details of raw and exported data formats are listed below.

equipment	raw format	exported format
New method developed in the project	CSV	CSV
Quartz crystal gravimetry	CSV	CSV
X-ray diffraction	XRDML	CSV
scanning electron microscopy	TIF or JPEG	
Transmission electron microscopy	TIF or JPEG	
Infrared spectroscopy	BSP	CSV
Nuclear magnetic resonance spectroscopy	FID	CSV
X-ray photoelectron spectroscopy	SPE	CSV
thermogravimetric analysis	NGB-SS3	CSV
mass spectroscopy	EXP	CSV
UV Vis spectroscopy	SP	CSV

Objective 2: Measure single- and multicomponent diffusivities even for fast-diffusing components details of raw format and exported format are listed below.

equipment	raw format	exported format
X-ray diffraction	XRDML	CSV
scanning electron microscopy	TIF or JPEG	
infrared spectroscopy	BSP	CSV
optical microscopy	TIF or JPEG	
Design files	Various proprietary formats	

Objective 3: Detect the presence of surface barriers

details of raw format and exported format are listed below.

equipment	raw format	exported format
New method developed in the project	CSV	CSV
Quartz crystal gravimetry	CSV	CSV
X-ray diffraction	XRDML	CSV
scanning electron microscopy	TIF or JPEG	
Transmission electron microscopy	TIF or JPEG	
Infrared spectroscopy	BSP	CSV
Nuclear magnetic resonance spectroscopy	FID	CSV
X-ray photoelectron spectroscopy	SPE	CSV
thermogravimetric analysis	NGB-SS3	CSV
mass spectroscopy	EXP	CSV
UV Vis spectroscopy	SP	CSV

3. LEGAL & ETHICAL ISSUES

Will you use personal data? If so, shortly describe the kind of personal data you will use (add the reference to your file in your host institution's privacy register - not relevant yet)

- 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 formal approval 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 what data and which restrictions will be asserted?

- Yes

If the proposed concept works, a meeting will be planned with the the KU Leuven tech transfer office to investigate patentability. The base technology of the approach is already protected by a granted patent. In case a patent application will be filed directly resulting from this project, the related data will not be freely shared at least until the patent filing.

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

- No

4. DOCUMENTATION & METADATA

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

An overview file that contains references to the raw data files will be kept. Regular reports based on the data will be generated using Microsoft Word. PowerPoint files will be used for presentation at regular internal meetings between the WP leaders and researchers involved in the project. In both the Word reports and Powerpoint presentations, the file names of the raw data files will be included.

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

- No

The details of each experiment will be kept in an electronic lab notebook. In this notebook, also the names of the raw and processed datafiles will be mentioned. Files will be named according to a pre-agreed convention. This working method obviates the need for a separate INFO.txt file in each directory yet ensures that the data can be understood by other team members and can be reused in the future. For published papers, the subset of the raw and processed data discussed in that manuscript will be copied and organized according the paper structure. Likely, this is the data subset that will be most frequently revisited and shared afterwards.

5. DATA STORAGE & BACK UP DURING THE FWO PROJECT

Where will the data be stored?

The data will be stored via a cloud storage solution that allows sharing with the WP leaders and researchers involved in the project.

How is back up of the data provided?

The data on the cloud storage server are automatically backed up. Unlimited versioning is included in the selected plan so that accidental erasing or modifying does not pose a risk.

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

The total amount of data generated during the project should not exceed a few TB and is therefore compatible with the selected cloud storage solution.

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

The costs for saving the data to the cloud storage server (including regular backup) should not exceed a few hundred euros. These costs will be covered by the project.

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

The data generated during the project will be systematically transferred to the cloud storage server. Only the WP leaders and researchers involved in this project will have access to the shared folders where the data, reports and presentations will be stored.

6. DATA PRESERVATION AFTER THE FWO 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 the reasons for this (legal or contractual restrictions, physical preservation issues, ...).

All the generated data will be stored on the cloud storage server for a period of 5 years after the end of the project.

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

All the generated data will be stored on the cloud storage server for a period of 5 years after the end of the project.

Beyond 5 years after the end of the project, one of the following options will be picked (1) continuation of storing the data on the cloud storage server or (2) transferring the data to the KU Leuven central servers for archiving.

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

The annual cost for long-term storage of the data, either through a cloud storage service or the university's central servers, is estimated at a few hundred euro. Since the budget of the current FWO project will no longer be available, creative solutions will have to be found.

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)?

- Yes. Specify:

The data will remain accessible among the WP leaders and the researchers involved in the project. Access to the data can be granted to other persons, upon request and agreement among the leaders. A patent application can be a limiting factor in granting access to the data.

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

In case no restrictions apply, the written reports and Powerpoint presentations summarizing the results obtained can be made available. The (raw) data used in publications can be made available on a repository, if e.g. requested by the Editors or Publisher of a scientific journal.

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

- Upon request by mail

The data that will not have been uploaded in a repository such as 'Scientific data' (<https://www.nature.com/sdata/>) to accompany a publication can be requested via email.

When will the data be made available?

- Upon publication of the research results

Description of the full scientific method and results will be made available with journal publications.

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

Upon request, access to the samples and data can be granted, upon agreement of the project leaders. Commercial reuse will not be allowed.

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

Because of the choice for a cloud storage solution for the data, no additional costs will be booked for data sharing.

8. RESPONSIBILITIES

Who will be responsible for data documentation & metadata?

The project leaders and the researchers involved in this project will be jointly responsible.

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

The project leaders and the researchers involved in this project will be jointly responsible. Because of the choice for a cloud storage solution, no additional action is needed for data backup.

Who will be responsible for ensuring data preservation and reuse ?

The project leaders and the researchers involved in this project will be jointly responsible.

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

The project leaders bear the end responsibility of updating & implementing this DMP.