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## Harnessing ion resource recovery: A multi-scale modelling strategy towards rational design of selective ion exchange membranes

*A Data Management Plan created using DMPonline.be*

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### Project abstract:

Critical materials such as lithium and cobalt are essential for developing green energy technologies (e.g., lithium-ion batteries). The rapid depletion of global reserves has shifted the focus of critical ion extraction towards recycling and sea mining, urging for more efficient & greener separation technologies. Selective electrodialysis using ion exchange membranes (IEM) emerges as a versatile technology for ion separation, but the lack of understanding on the separation mechanisms hinders further development of target-ion selective IEMs that can achieve one-step purification. Thus this project aims to establish a multi-scale modelling strategy towards rational design of ion-selective IEMs, via a combined modelling & experimental approach. Here four interactive work packages are designed: the first two will focus on building a preliminary and advanced model of non-selective IEMs, aiming to understand the model applicability & influence of non-ideal transport factors that may compromise performance. The third will establish new correlations of transport rate-controlling parameters that bridge micro- & macro-level properties of the separation. As a result, a white-box continuum model will be developed & demonstrated via experimental membrane optimization. Such mechanistic model is expected to serve as an important toolkit to guide membrane design, making electro-driven membrane technology a viable option for critical ions/minerals recovery for sustainable energy applications.

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### DPIA

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#### DPIA

Have you performed a DPIA for the personal data processing activities for this project?

- Not applicable

## Harnessing ion resource recovery: A multi-scale modelling strategy towards rational design of selective ion exchange membranes

### GDPR

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#### GDPR

Have you registered personal data processing activities for this project?

- Not applicable

## **Harnessing ion resource recovery: A multi-scale modelling strategy towards rational design of selective ion exchange membranes**

### **Application DMP**

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#### **Questionnaire**

**Describe the datatypes (surveys, sequences, manuscripts, objects ... ) the research will collect and/or generate and /or (re)use. (use up to 700 characters)**

The expected types of data generated from this research are publishable research manuscripts and patents. The original data may consist of the experimentally acquired values (e.g., lab books, .txt, .csv) and computational codes/programs (e.g., MATLAB, .txt) in the chemical engineering domain, these however may be reused for future research development. Nevertheless, not all data will be kept beyond the lifetime of the proposed project, such as invalid data (that is not reproducible), and data that can contribute to the public knowledge domain, e.g., as journal publications and for education training purposes. Overall, there is no personal data involved.

**Specify in which way the following provisions are in place in order to preserve the data during and at least 5 years after the end of the research? Motivate your answer. (use up to 700 characters)**

During the research, the data will be stored in the university's central network drives as they are safe and automatically backed up. Sensitive data will not be carried on unprotected personal devices.

When the research project ends, there are a few options to preserve the data for minimum of 5 years, such as KU Leuven/UZ Leuven servers, archiving and/or share/publish data. Also, we can make use of the general repositories such as Harvard's Dataverse and internal KU Leuven repository (i.e., Lirias).

**What's the reason why you wish to deviate from the principle of preservation of data and of the minimum preservation term of 5 years? (max. 700 characters)**

There will be two possible reasons that deviation from the 5-year principle will apply: the use of personal data or the restriction imposed by 3rd parties. In this project, the first case is not applicable.

**Are there issues concerning research data indicated in the ethics questionnaire of this application form? Which specific security measures do those data require? (use up to 700 characters)**

Not Applicable

**Which other issues related to the data management are relevant to mention? (use up to 700 characters)**

Not Applicable

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FWO DMP (Flemish Standard DMP)

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## 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
		<i>Please choose from the following options:</i> <ul style="list-style-type: none"> <li>• Generate new data</li> <li>• Reuse existing data</li> </ul>	<i>Please choose from the following options:</i> <ul style="list-style-type: none"> <li>• Digital</li> <li>• Physical</li> </ul>	<i>Please choose from the following options:</i> <ul style="list-style-type: none"> <li>• Observational</li> <li>• Experimental</li> <li>• Compiled/aggregated data</li> <li>• Simulation data</li> <li>• Software</li> <li>• Other</li> <li>• NA</li> </ul>	<i>Please choose from the following options:</i> <ul style="list-style-type: none"> <li>• .por, .xml, .tab, .csv, .pdf, .txt, .rtf, .dwg, .gml, ...</li> <li>• NA</li> </ul>	<i>Please choose from the following options:</i> <ul style="list-style-type: none"> <li>• &lt;100MB</li> <li>• &lt;1GB</li> <li>• &lt;100GB</li> <li>• &lt;1TB</li> <li>• &lt;5TB</li> <li>• &lt;10TB</li> <li>• &lt;50TB</li> <li>• &gt;50TB</li> <li>• NA</li> </ul>	
Ion Exchange Membrane Models	Non-selective models (with and without non-ideality) and selective model	Generate new data	Digital	Simulation data	.mph, .docx, .xlsx	<1TB	
MATLAB Codes	Codes for sensitivity analysis, non-ideal transport correlations, theoretical activation energies, and optimization modules	Generate new data	Digital	Simulation data	.m, .docx, .xlsx	<100MB	
ICP-OES	For ionic concentrations	Generate new data	Digital	Experimental	.xlsx	<100MB	
Microscopy Images	Microscopic images of the structure of membranes	Generate new data	Digital	Experimental	.tiff	<1TB	
Fourier Transform Infrared Spectroscopy	Qualitative surface chemistry analysis of membrane samples	Generate new data	Digital	Experimental	.tiff	<1GB	
Notes	Electronic Lab notebook	Generate new data	Digital	Compiled/aggregated data	.docx, .xlsx, .pdf	<100MB	
Manuscripts	Written texts/scientific publications	Generate new data	Digital	Compiled/aggregated data	.docx, .pdf,	<1GB	
Presentations	Slides and presentation notes	Generate new data	Digital	Compiled/aggregated data	.ppt, .pdf,	<1GB	

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).

- **Ion Exchange Membrane Models:** These CFD models will be constructed using COMSOL software. For each model, multiple simulations files of .mph format will be generated with labelling ("WPnumber\_modelname\_conditions"). Moreover, .docx file will be made to accompany each model file and will contain all the simulation conditions and observations and .xlsx files for output plots and graphs.
- **MATLAB Codes:** These codes will be constructed using MATLAB software. For each workpackage that requires coding, different script files of .m format will be generated with labelling ("WPnumber\_modelname\_correlationtype"). Moreover, .docx file will be made to accompany each code file and will contain all the simulation conditions and observations and .xlsx files for output plots and graphs.
- **ICP-OES:** Samples are prepared according to SOPs and named "name\_D/C\_time". 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.
- **Microscopy Images:** Pictures are taken according to SOPs, saved in .tiff and named "name\_type\_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.

- **Fourier Transform Infrared Spectroscopy:** Samples are prepared according to SOPs and named "name\_type\_conditions". Observations and procedures are digitally reported in a lab notebook. After operation, samples are not stored but can be partially recuperated.
- **Notes:** The electronic lab notebook is used for setup design (sketches) and writing down of observations. This notebook will be stored in KU Leuven drives.
- **Manuscripts:** Communication of scientific results is done via manuscripts and saved in .docx, .pdf or .tex.
- **Presentations:** Presentations containing scientific results are produced using PowerPoint and stored accordingly (.ppt or .pdf).

**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 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.

#### **How will the data be backed up?**

Data are backed up on the cloud (OneDrive) immediately. The software indicates the update status (green, blue or red) and, in case of a non-sync, action can be taken using the online version of the tool. Data are further back up regularly on an external hard drive. After completion of (sub)WPs, data will be additionally backed up on 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. Xing Yang.



#### 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 the data will be retained for the expected 5 years period after the end of the project with no exceptions.

**Where will these data be archived (stored and curated for the long-term)?**

All the data will be stored for the long-term on the KUL service 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 expected costs of data storage and preservation are around €5000. These costs will be covered by Prof. Xing Yang

#### 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, ...)

Data relevant for publication will be made available in an Open Access repository (i.e., Lirias). Full datasets will only 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 (i.e., Lirias). 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 findings.

**Which data usage licenses are you going to provide? If none, please explain why.**

For Ion Exchange Membrane Models: COMSOL license will be provided with the appropriate modules.

For MATLAB Codes: MATLAB License will be provided

**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 tools like Belnet FileSender (KUL account) will be used for data sharing. In the unlikely event that there would be costs, these costs will be covered by Prof. Xing Yang.

## **6. Responsibilities**

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

Omar Elshawarby

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

Omar Elshawarby

**Who will manage data preservation and sharing?**

Prof. Xing Yang

**Who will update and implement this DMP?**

Omar Elshawarby and Prof. Xing Yang bear the end responsibility of updating and implementing this DMP in the long term.