Tailoring membranes for sustainable molecular separations: preparation and multi-scale modelling

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Project abstract:

Separation processes account for ~50% of industrial and ~15% of the global energy consumption. Improving the energy efficiency of these processes thus grants enormous economic and environmental benefits. Compared to conventional technologies, **membrane technology could save up to 90-99% energy for many key applications**. In addition, **no waste streams** are being generated and membrane separations also possess a **small footprint and modular design**, allowing easy retrofit in existing plants. Nevertheless, the lack of membranes with high performance and sustained stability over an extended operational period is a major obstacle in the field.

Gas separation is one of the most challenging and energy-intensive separations. Membranes are quite well applied already in, e.g., natural gas purification, H2 recovery and air separation and will be crucial to CO2 capture for realizing a carbon-neutral future. However, current polymeric membranes tend to suffer from intrinsic permeability/selectivity trade-offs or plasticisation, which causes significant deterioration in membrane selectivity in presence of even trace amounts of certain compounds in the processing streams (e.g., water vapor or hydrocarbons).

Other highly relevant separations relate to **liquids,** such as in crude-oil separations or fine chemical and pharma applications (e.g. product removal from reagents and catalysts). The potential market size for membrane separations in these applications is huge. So called solvent-resistant nanofiltration (SRNF) could well replace the current energy-intensive distillation or waste-intensive crystallization, preparative chromatography processes. Also here, there is still a clear need for membranes that remain stable in these harsh streams and that combine good selectivity with sufficient permeation.

In both membrane-based gas and liquid separations, there is a **lack of fundamental theories** to link the membrane chemical/structural characteristics with the non-ideality of multi-component fluids, not to mention the lack of comprehensive **models** for predicting the separation behavior of a target compound from mixed streams, where the presence of co-existing components/impurities may adversely impact the membrane stability, or competitively transport through the membranes. Also, the inappropriate choices of operating conditions and module configurations may hamper the separation driving force. These phenomena may result in failures in membrane operation and limit scalability, thus should be systematically investigated for the design of future membranes and membrane systems.

This C1-project aims at (1) tailoring **new membrane materials** for these applications and at (2) enhancing the fundamental understanding of the final processes via **mathematical modelling** at two levels. (1) **Molecular tuning** of the polymers that form the membranes will allow optimization of the materials for the different gas and liquid applications, while (2) **module construction** will bring these materials to a final product that is closer to real applications. At both levels, material development and modelling will go hand-in-hand and offer directions for mutual improvement via feedback loops, in which modelling will guide membrane design and predict performances.

The **base hypothesis** of this proposal is that two, so far hardly explored, polymer types (i.e. **polycarbonates and epoxide-based polymers**) can help solve the above application issues. Thanks to the postdoctoral stay of Rhea Verbeke at Prof. Frey's research team at Mainz University (Germany) where novel types of these polymers have recently been developed, a whole platform of novel, tunable membrane polymers has come in reach. Monomers, many of them bio-based, will thus be selected to manipulate the polarity, crosslinking degree and charge of the final polymer. The resulting membranes will then be applied in a selection of gas and liquid separation where optimal molecular interactions between the functional groups of the polymer and the permeating compound will be realized. Polymer crosslinking will enhance membrane stability and create stable performance. Charges will further enhance molecular

discrimination and incorporation of porous, selective fillers will further expand the toolbox. The tuned materials will then be brought to the more practical level by constructing modules with the resulting membranes. To more **rationally design** these membranes, this project will also establish a fundamental framework via a novel **multi-scale modeling** strategy to understand the key performance limiting factors in these membranes and separation processes, by combining the power of the molecular dynamic (MD) simulation and computational fluid dynamic (CFD) modeling. On molecular level, the interfacial properties of the membrane will be quantified considering the diffusion and sorption kinetics of each component and membrane surface chemistry. The interaction between models of two levels will yield a comprehensive continuum model to account for the non-ideality of fluid properties, dynamic membrane characteristics linked to material deterioration, and flow dynamics linked to module configuration.

The success of this project will produce **rationale routes for designing high-performance membranes and membrane-based systems**, addressing fundamental challenges faced in many fields such as environmental, chemical purification, and energy production.

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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	
Lab notes	Description of the practical execution of experiments	New	Digital and if Physical, they will be digitalized as materials and method section	Observational and experimental	.docx	<100 GB	5-10 note books
UV-vis	UV-vis spectra	New	Digital	Experimental	.xlsx	< 100 GB	
Filtration results	Results form the filtration experiments	New	Digital	Experimental	.xlsx	< 100 GB	
Literature	Background literature	Existing	Digital	Other	.pdf	< 100 GB	
IR	infrared spectroscopy data	New	Digital	Experimental	.xlsx/.dpt/.0	< 100 GB	
Density measurements	Density measurement data	New	Digital	Experimental	.xlsx	< 100 GB	
PALS	Positron annihilation lifetime spectroscopy	New	Digital	Experimental	.xlsx	< 100 GB	
Gas adsorption	Gas adsorption experiment data	New	Digital	Experimental	.xlsx	< 100 GB	
XPS	X-ray photoelectron spectroscopy data	New	Digital	Experimental	.xlsx	< 100 GB	
ERD	Elastic recoil detection data	New	Digital	Experimental	.xlsx	< 100 GB	
Porometry	Porometry data	New	Digital	Experimental	.txt/.xlsx/.docx	< 100 GB	
Microscopy data	SEM, TEM, AFM	New	Digital	Experimental	.tif	< 100 GB	
Modeling data	DFT, molecular simulations, CFD	New	Digital	Simulation	.mat / .txt /.top /.JPG /.png /.gif	< 1 TB	

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:

N.a.

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

Before every publication, the potential towards IP creation will be assessed. If there is IP potential, the relevance will be communicated with the relevant tech transfer offices. Therefore, all relevant data will be kept restricted until assessment towards filing a patent. Once these granted, this data can be made public.

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).

The data files will be named using a standardized naming system, including date of the experiment, name of the researcher, sample code,... The used codes will correspond to the codes used in the lab notebooks.
An index or table of content file will be provided with the explanation of each code and a short description of each related project. In this index, also a link will be embedded to the data file location.

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?

- Shared network drive (J-drive)
- OneDrive (KU Leuven)

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?

Data will only be stored on OneDrive and the internal KU Leuven drives. Both are only accessable through a 2-step autentication protocol (password and KU Leuven authenticator).

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

The costs for storage on the shared J: drive are 500 euro/TB. OneDrive is free of charge.

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)

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

The costs for long term data storage are 50 euro per TB per year.

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)

If access is restricted, please specify who will be able to access the data and under what conditions.

All researchers and PI will have access at all time to the data. Externals can get access to the data upon approval of the PI.

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.

- Yes, intellectual property rights

Only data with potential IP protection will be restricted to the consortium members and will not be published before filing a patent.

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.

- Data Transfer Agreement (restricted data)
- CC-BY 4.0 (data)

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?

KU Leuven RDR free for 50 GB

Responsibilities

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

The researchers

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

The researchers

Who will manage data preservation and sharing?

Ivo Vankelecom, Xing Yang and Laurens Rutgeerts

Who will update and implement this DMP?

Laurens Rutgeerts