Organic Solvent Nanofiltration and Data-Driven Approaches

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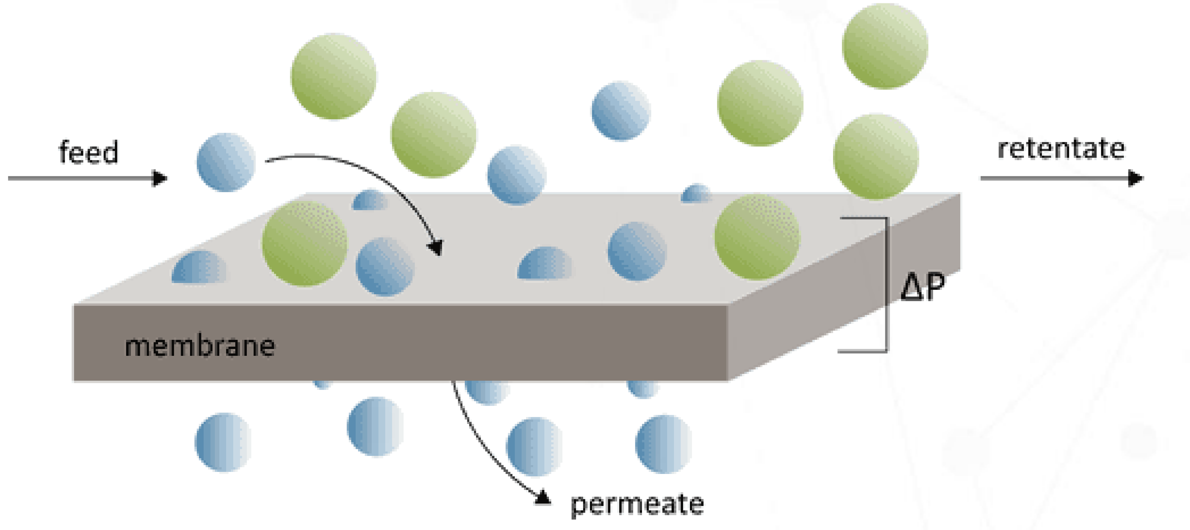
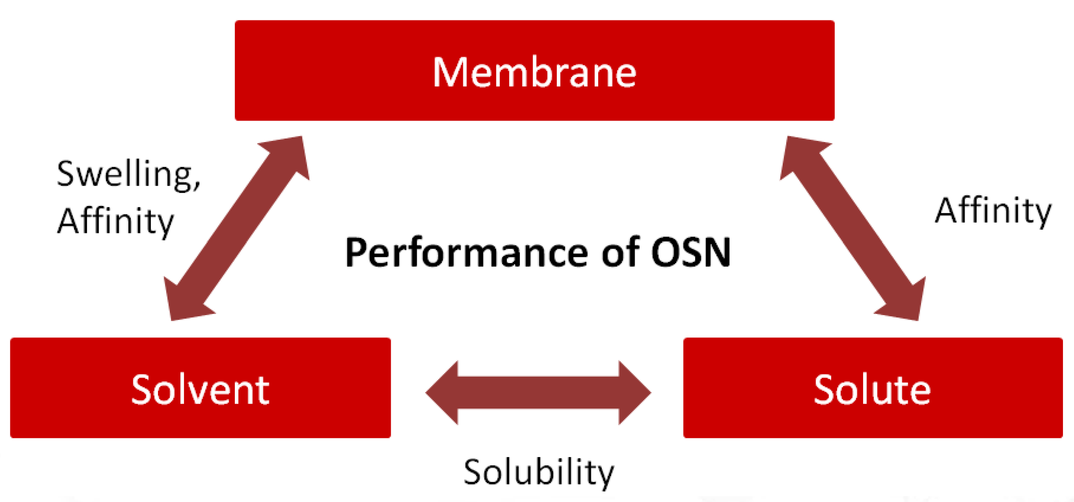
Problem Statement

Membranes are powerful, versatile separation tools, offering an energy-lean alternative for traditional thermal separation methods.



However, due to the complexity of this membrane process, influenced by all mutual solute–solvent–membrane interactions and properties, the **transport mechanism is not well understood**. This leads to a slow, trial-and-error based development process.



To **speed up the development process**, and to try and understand the separation mechanism, we resort to **data science**.

Physical models

Physical transport models exist but were originally developed for water filtration. Since they **link physics to membrane performance**, these models can be used to investigate the underlying physics. A review was published on physical models and data-driven modelling in the field [1].

Review

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The Database

Data structure is complex:

- **Highly dimensional** (over 30 features)
- Still small amount of data available (500 points)

→ Creating data-driven models is challenging

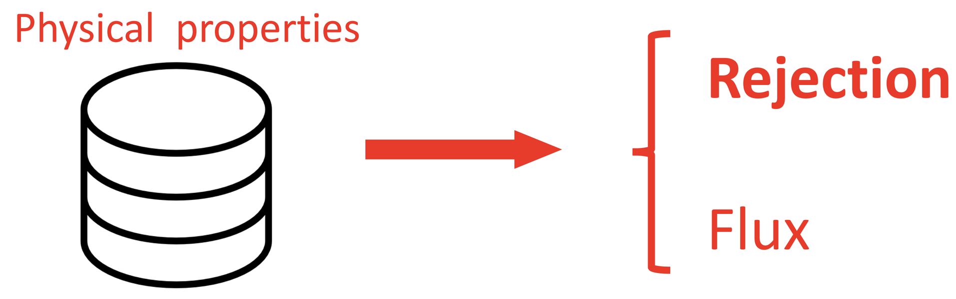
Unique database:

- **Ceramics**
- Cross-flow focused
- Unprocessed data to be added (~10 000 points)

Data science

Currently, **exploratory data-analysis** is ongoing. Among exploration of data, techniques include correlations (e.g. PCA).

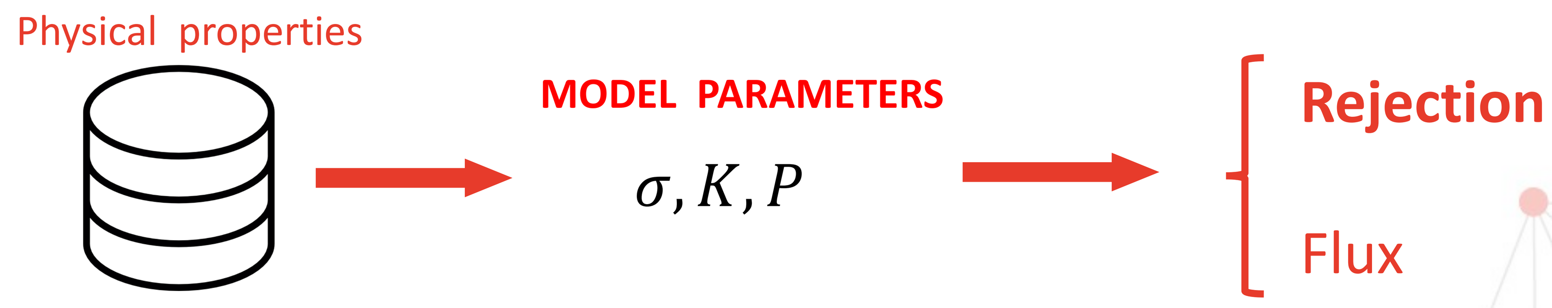
Thereafter will follow the creation of **data-driven models** to predict the separation performance from the physical properties.



Techniques for data-driven modelling include:

- Linear regression
- Gradient boost
- Neural networks

A future step is to model via physical models to **gain physical insight** by linking physical properties to model parameters.



References & Acknowledgement

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[1] P.-J. Piccard et al., Separations 2023, doi: 10.3390/separations10090516