Organic Solvent Nanofiltration and Data-Driven Approaches

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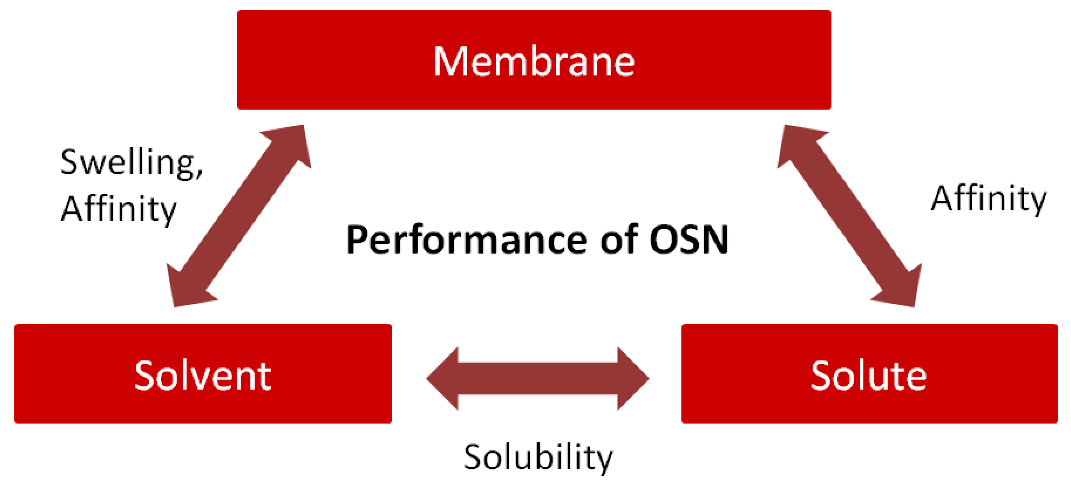
Problem Statement

Due to the complexity of the membrane separation 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**.

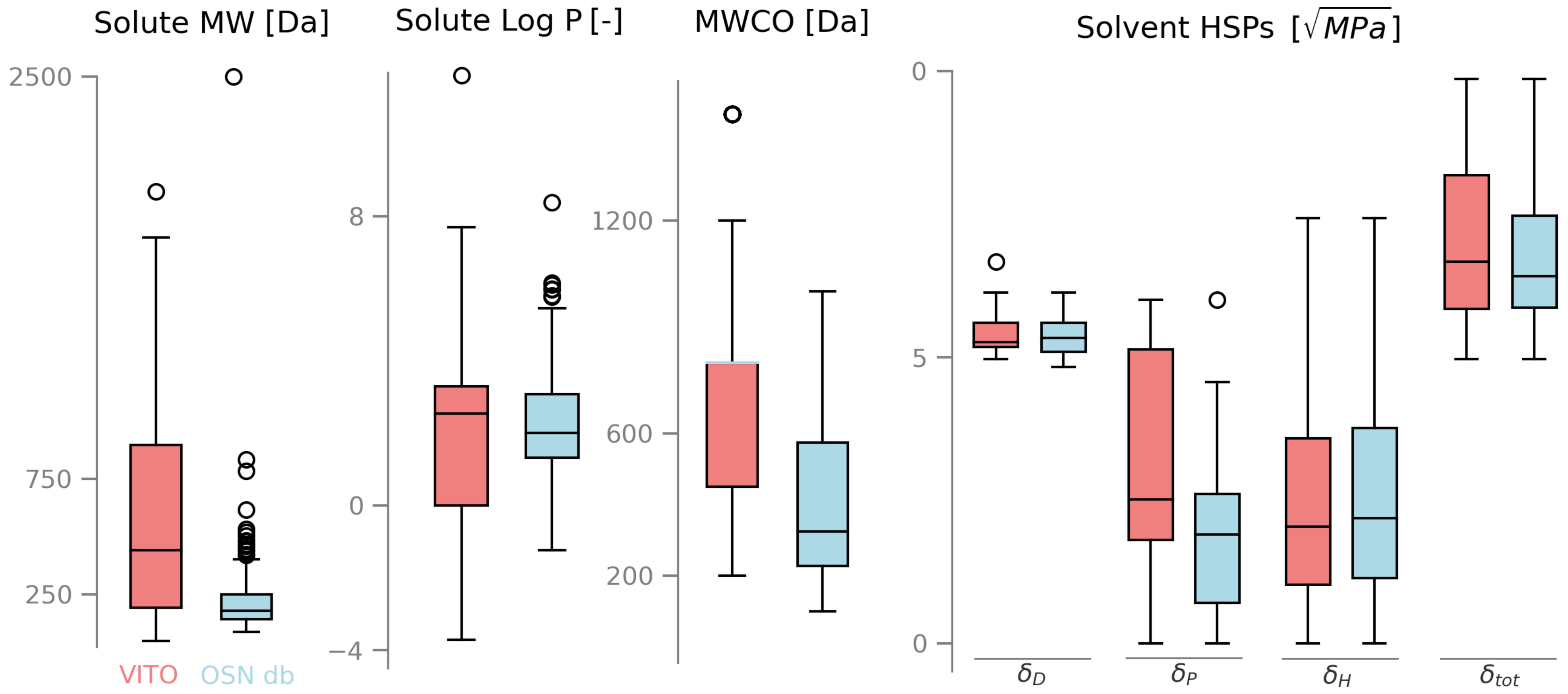


Unique Database

Filled with **Ceramics:**

- Native + Grafted
- Cross-flow focused
- **No Swelling**

Currently 1000 data points available, but still ~10 000 points of data to be added.



Comparing the content of the databases of **VITO** and **OSNdb**.

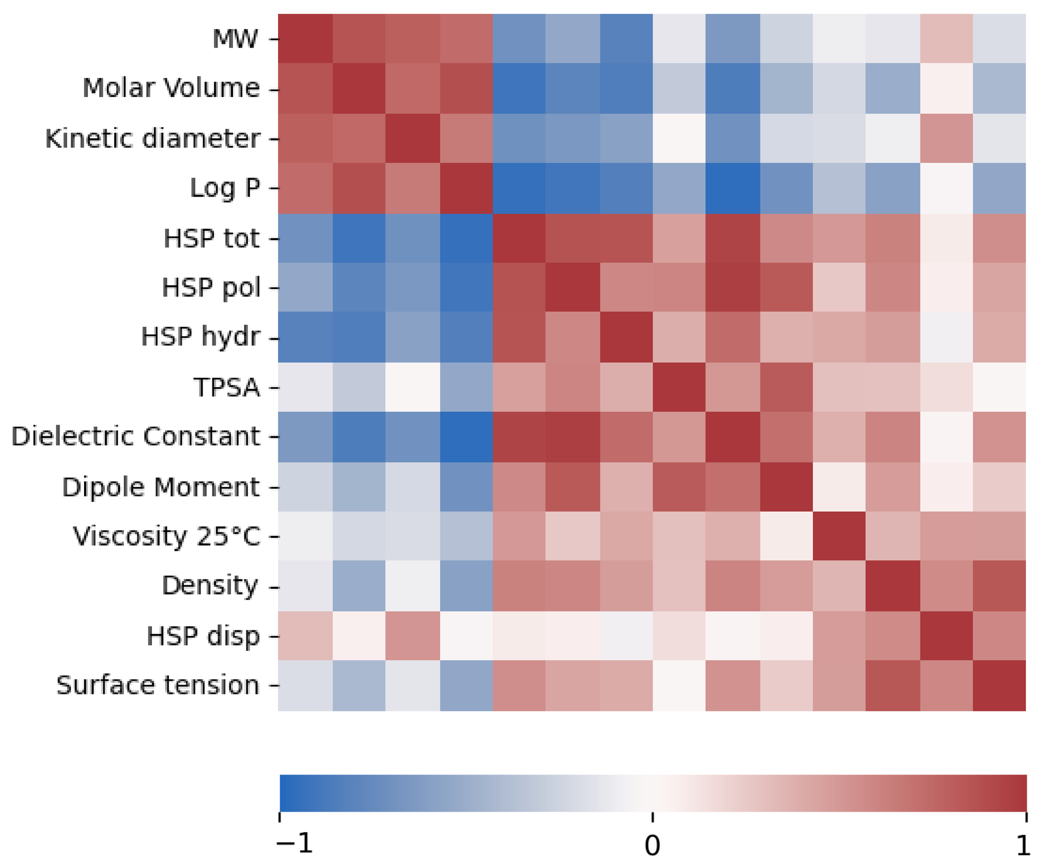
(see OSNdb.KAUST.edu.sa)

VITO's more hydrophilic, ceramic membranes allow for a **broader range** in solvent and solute polarities. Note the relatively broad range in MWCO and solute MW as well.

Data Science

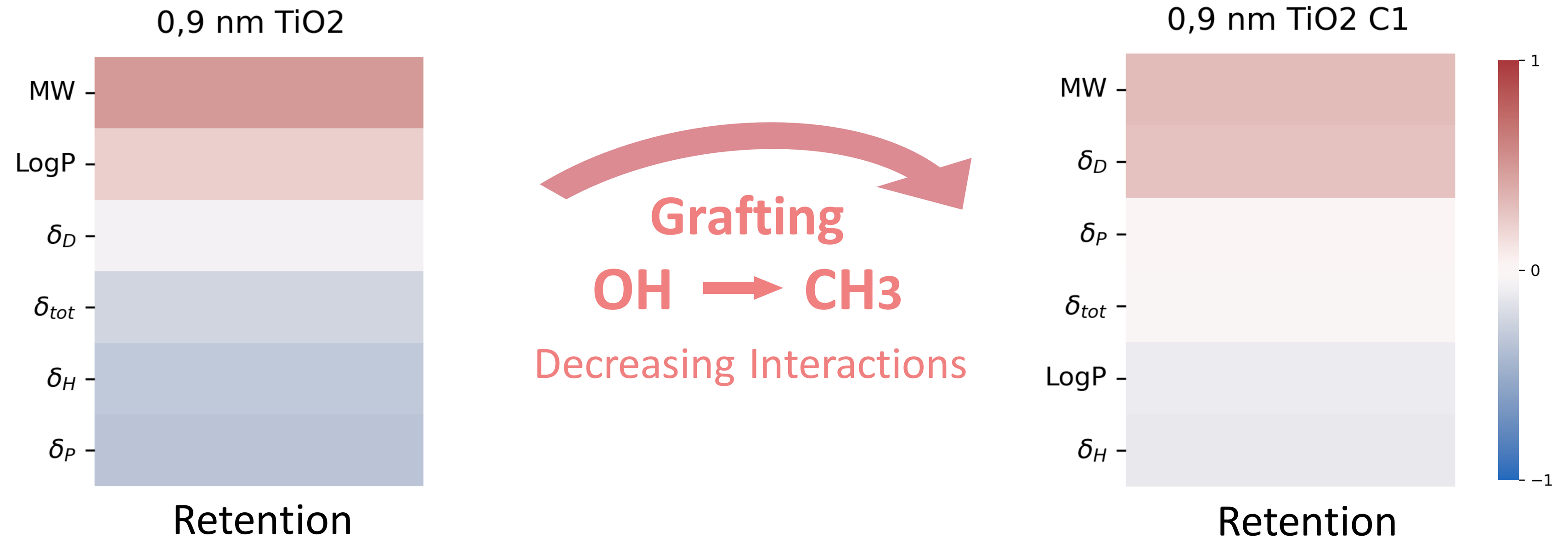
Currently, **exploratory data analysis** is ongoing. Techniques include PCA and exploration of correlation matrices.

Correlation Matrix of Solvent properties:

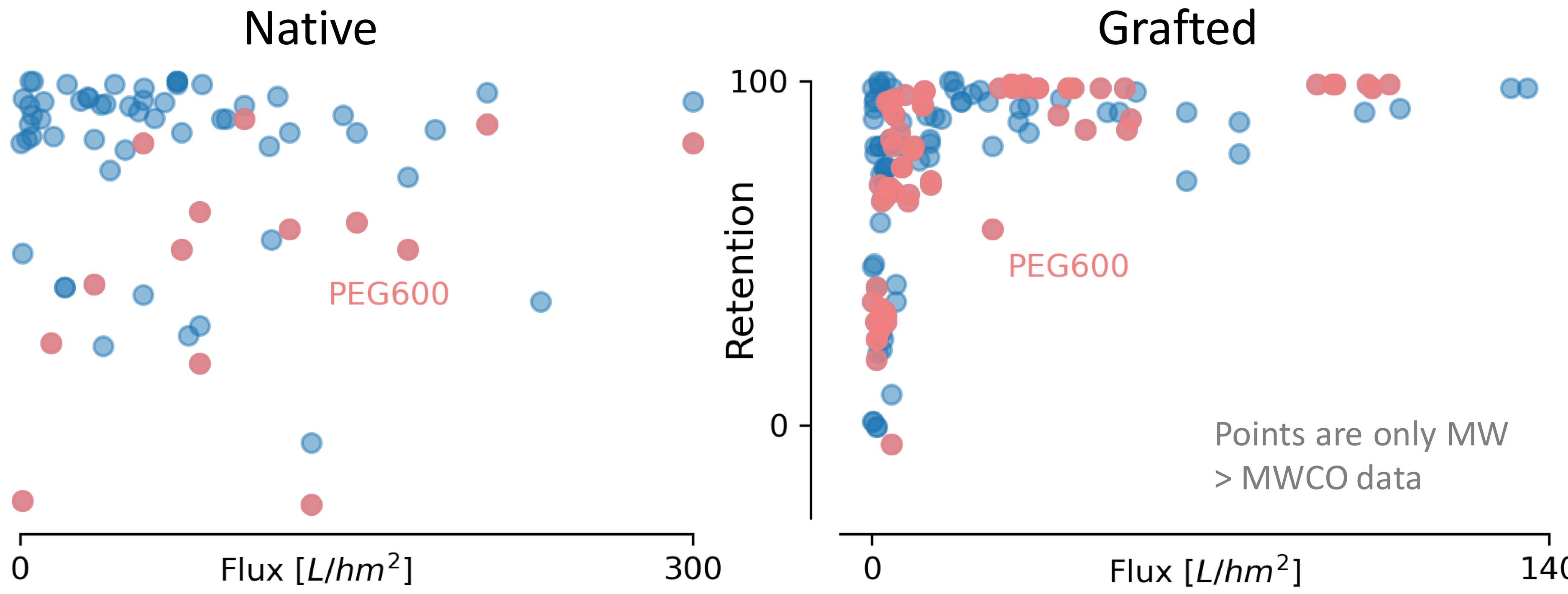


Determination of the most important descriptors are guided by unsupervised data analysis (dimensional reduction).

Correlating descriptors to retention gives **insight on the separation**:



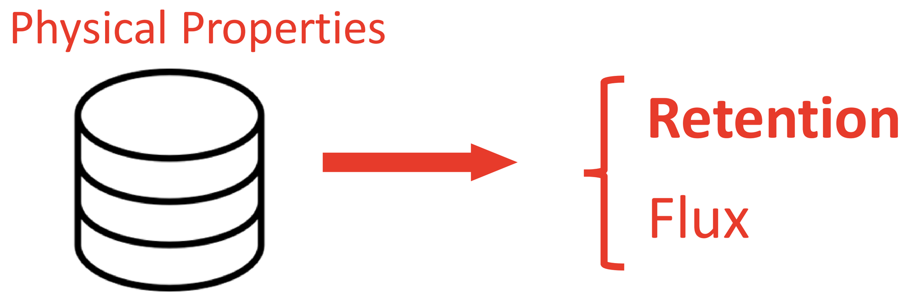
Retention in ceramic membranes is influenced by the solute polarity. Grafting them to more hydrophobic membranes reduces this effect.



Remarkably regular behavior is observed in the grafted membrane (right). This is likely explained by a difference in transport behavior.

Outlook

Create **data-driven models** to predict the separation performance from the physical membrane-solvent-solute properties.



A further step is to predict through mechanical models in order to **gain physical insight** by linking physical properties to model parameters.

Corresponding to the talk "Possible routes in data-driven approaches for ceramic membranes" by Jef Hooyberghs.

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Further reading: P.-J. Piccard et al., Separations 2023, doi: 10.3390/separations10090516