Predicting Ceramic Membranes Performance in Organic Solvent Nanofiltration: A Physics-guided Machine Learning Approach

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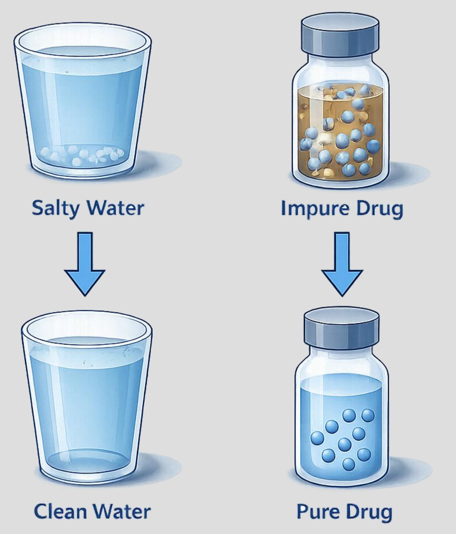
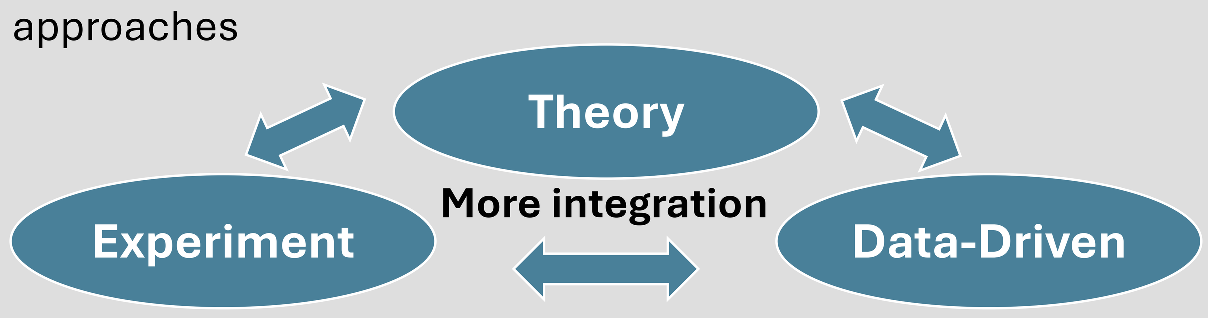
Introduction

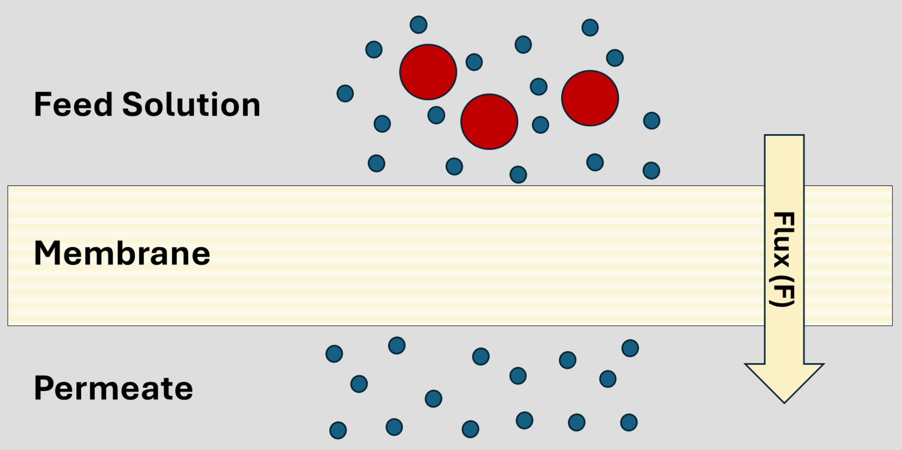


- **Separations** are everywhere (drug purification, water filtering, …)
- Most often: thermal separations like distillation
  → Require a lot of energy
- **Pressure-driven membranes** are an environmentally friendly and economical interesting alternative

- Industrial adaptation hindered by the research cost of identifying the right membrane for the job
  → Screening process
- Our research: **Predicting Membrane performance** through closer integration between theory, experiment and data-driven approaches



Membrane separation



Theory

Spiegler-Kedem model:

$$F = L_p(\Delta p - \sigma \Delta \pi) \quad (1)$$

$$R = \frac{\sigma(1 - e^{F(1-\sigma)/P_s})}{1 - \sigma\, e^{F(1-\sigma)/P_s}} \quad (2)$$

+ Good consistency with data

- Still relies on empirical parameters

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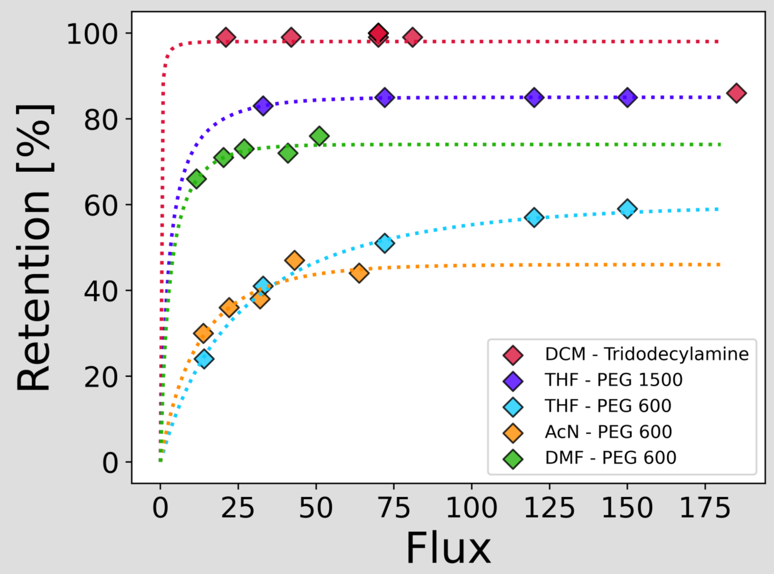
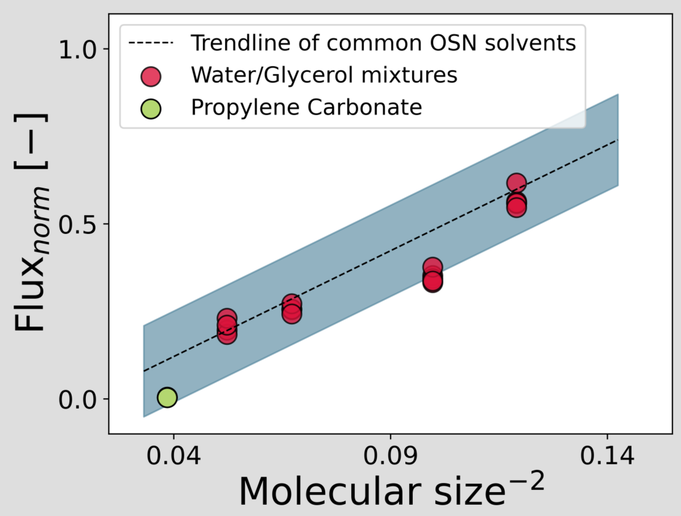
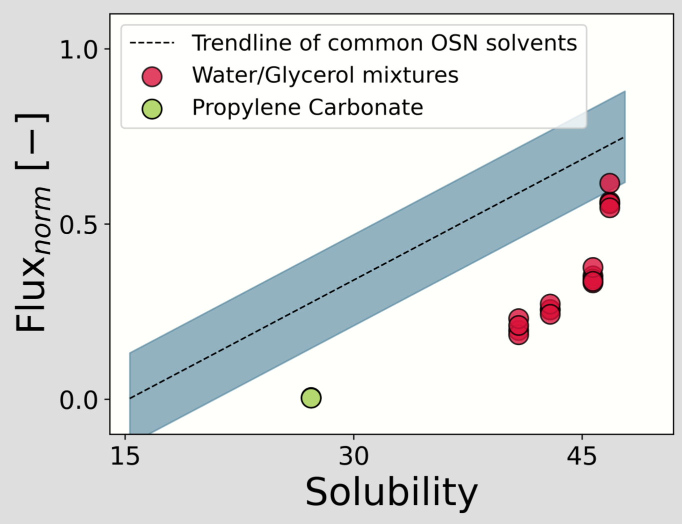
Embed within Deep Neural Networks:

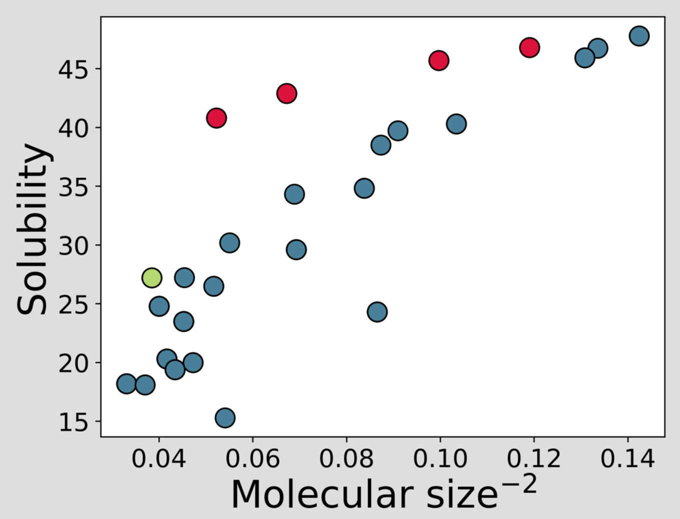
- Restrict dimensionality
- Keep physically relevant



Experimental - Breaking collinearity







- Both size and solubility seem to be good predictors of flux for common OSN solvents
- Interpretation complicated by **collinearity of descriptors**
- Break this with outlier solvent
- Molecular size poses the trend with flux while solubility was a **spurious correlation** with flux

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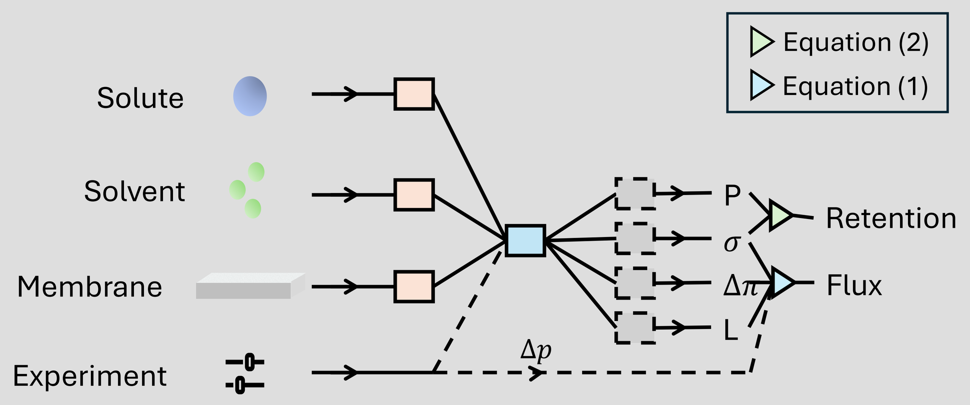
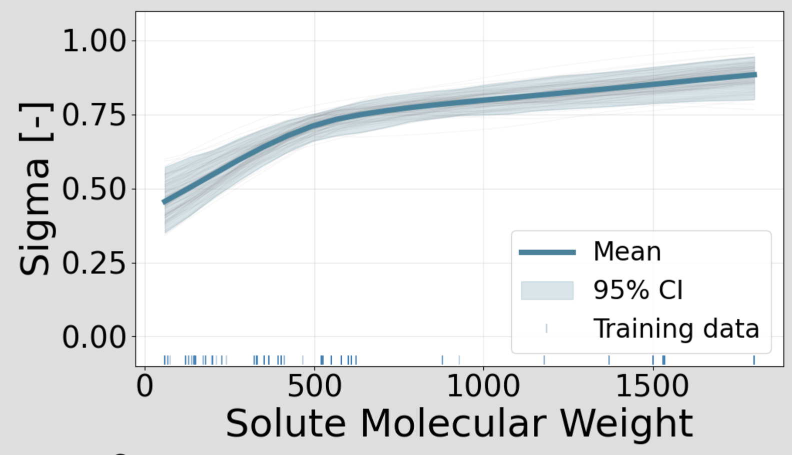
Data Driven – Explainable AI

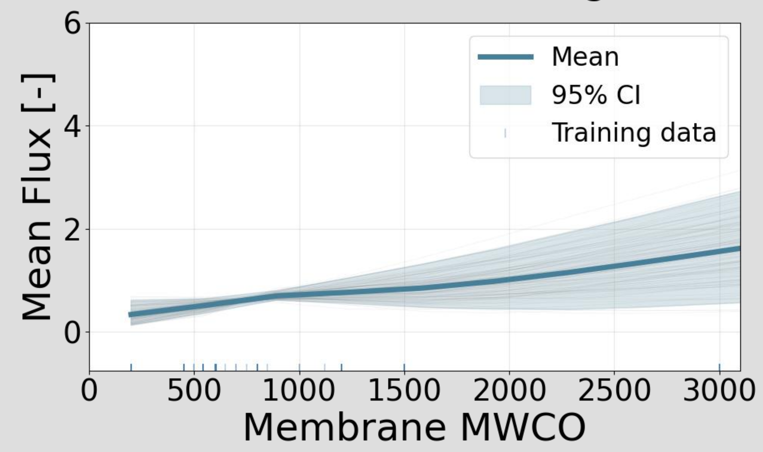


- PGNN (physics guided neural network) to predict Spiegler-Kedem parameters
- **Calculate retention and flux from predicted Spiegler-Kedem parameters**

- PGNN is a black-box model
- XAI to determine how the model made its prediction, on which features it relies
- Partial Dependence Plots (PDP) make it possible to **investigate dependencies between input features and the physical/target parameters of the PGNN**

→ Modeling membrane separations is possible with PGNN's and can be interpreted with PDP.





Outlook

- Membrane Selection and development trough **reversed modeling**
- **Energy Savings**: A transition to OSN can lead to an estimated 50-90% reduction in energy consumption compared to traditional distillation
- **Time-to-Market**: Reducing the experimental screening phase from months to days through predictive modeling
- **Integration** in standard industrial process simulators like Aspen Plus

References

[1] Piccard et al., *"Exploratory data analysis reveals the impact of solvent and solute on the performance of native and grafted ceramic membranes in organic solvent nanofiltration,"* **JOMS**, **735** (2025) 124509.

[2] Linsen et al., *"Decoupling solvent features to address spurious correlations in ceramic organic solvent nanofiltration membranes,"* **JOMS Letters**, **6**(1) (2026) 100111.

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