

Application of Machine-Learning Methods in Membrane Modification



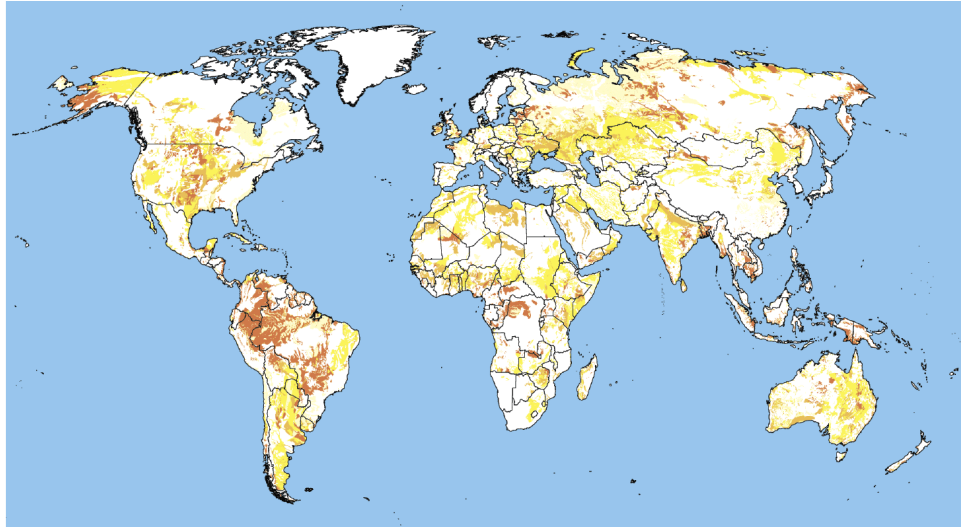
Dr. Sarah Glaß

Hereon-Institute of Membrane Research
Department of Microporous Polymers

MSE Days 2024, 5.11.24, Jülich

Introduction

Motivation

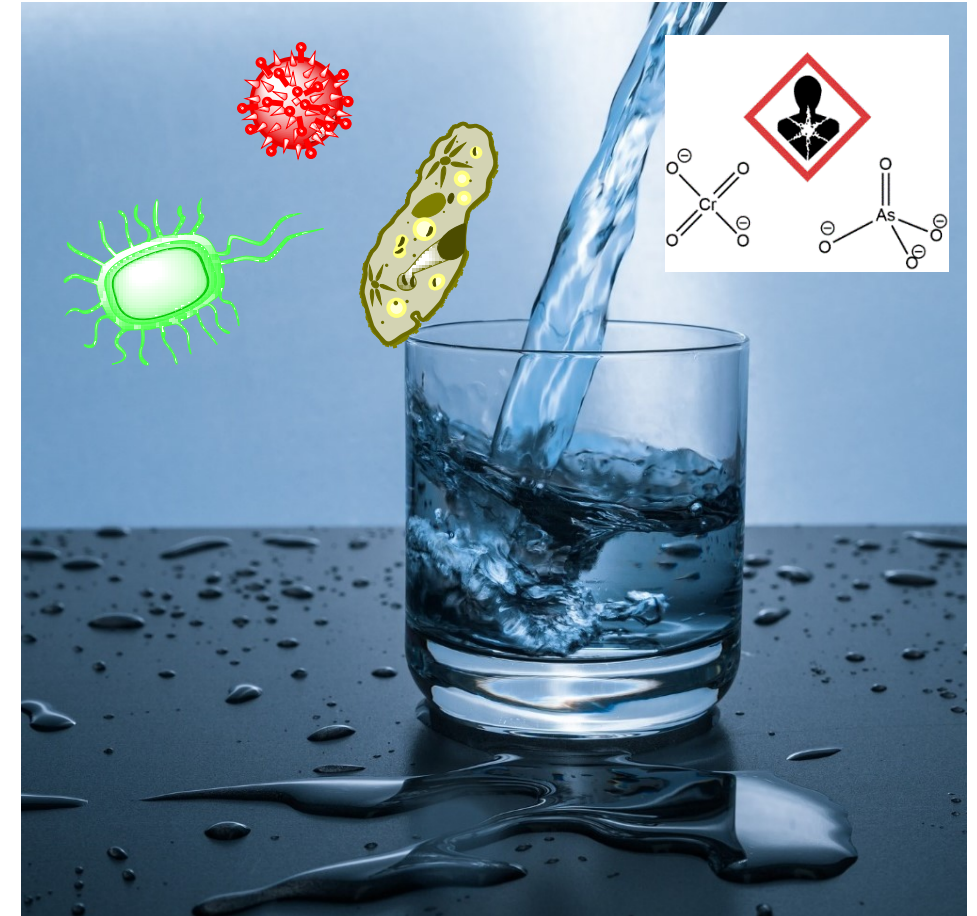


Wahrscheinlichkeit
Arsen > 10 µg/l

- 0 – 25 %
- 25 – 50 %
- 50 – 75 %
- 75 – 100 %

- Purification of drinking water

- Microbiologically safe (free of bacteria etc.)
- Free of heavy metals (arsenate, chromate)

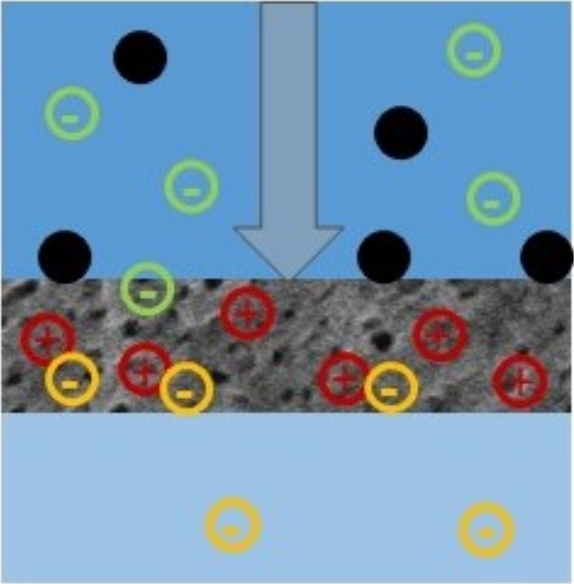


<https://www.wassertest-online.de/blog/wp-content/uploads/2017/08/Zink-im-trinkwasser-01.jpg>

Introduction

Motivation

Adsorption



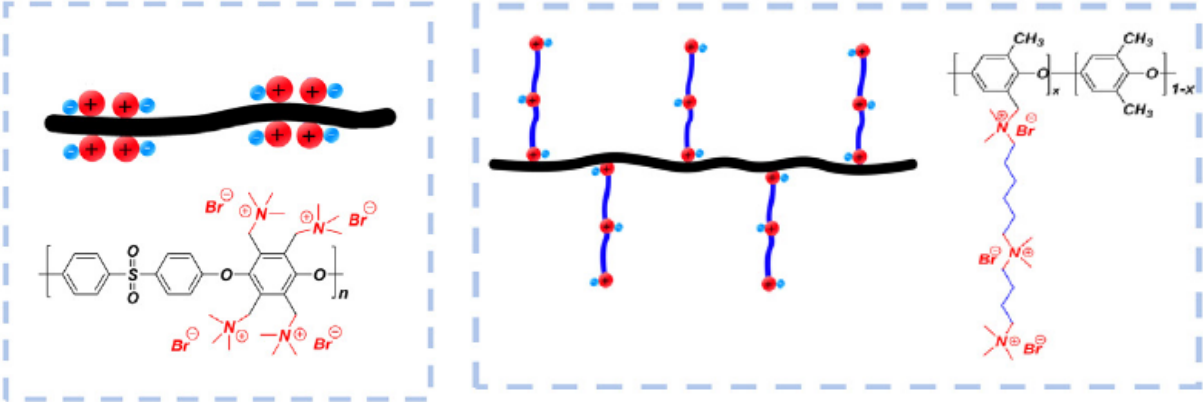
Toxic arsenate anions

Non-toxic chloride anions

Particles/Bacteria

Postmodification of Ultrafiltration Membranes

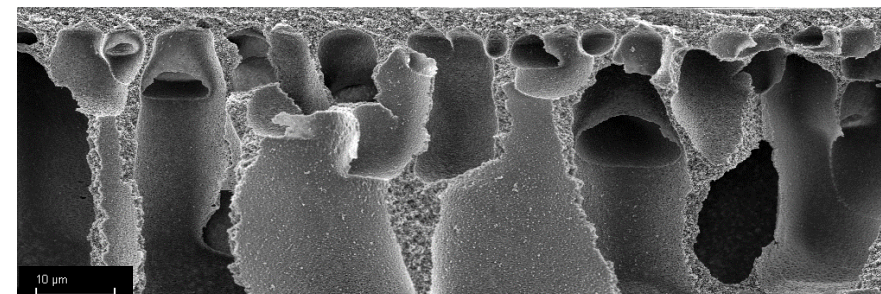
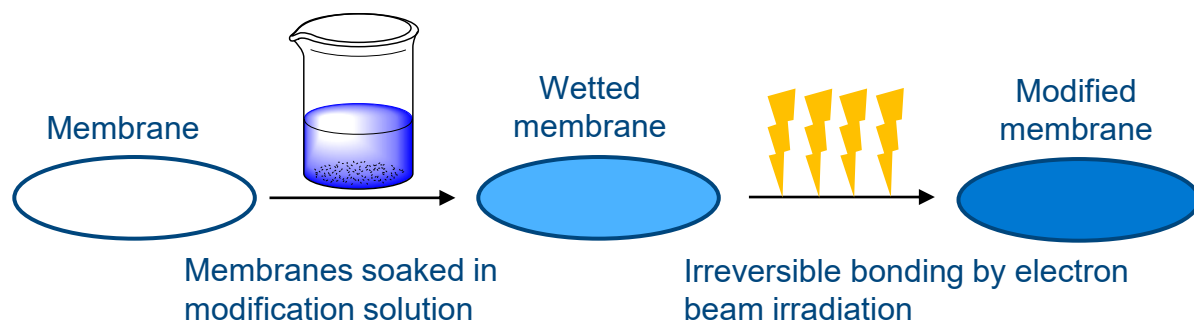
- Can be operated at low TMP (<0.5 bar)
- Flexible introduction of different adsorbing chemical groups
 - Positive Charges by usage of amine groups
 - Functional groups covalently bond to polymer



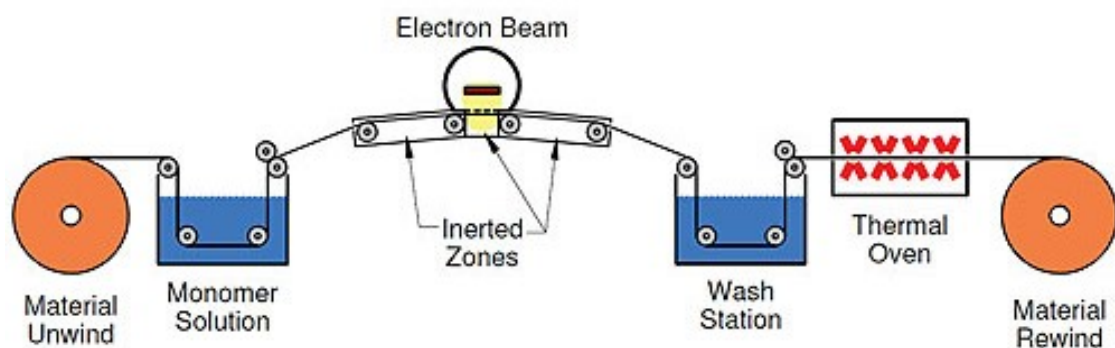
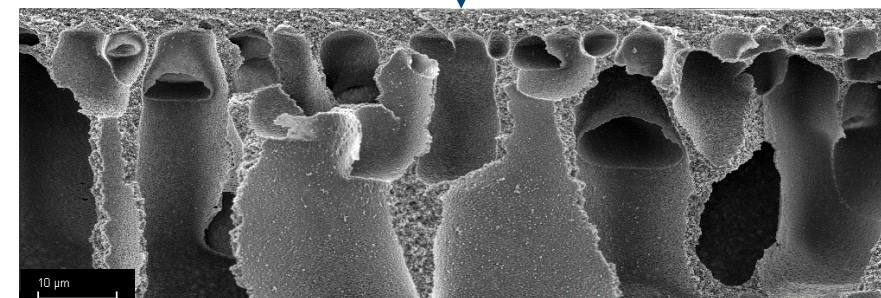
Modification strategy

Electron beam modification

Background electron beam modification



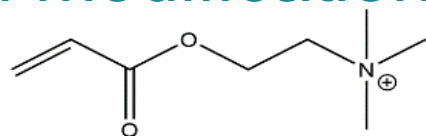
Amine containing
(hydrogel-) coating
with positive charge



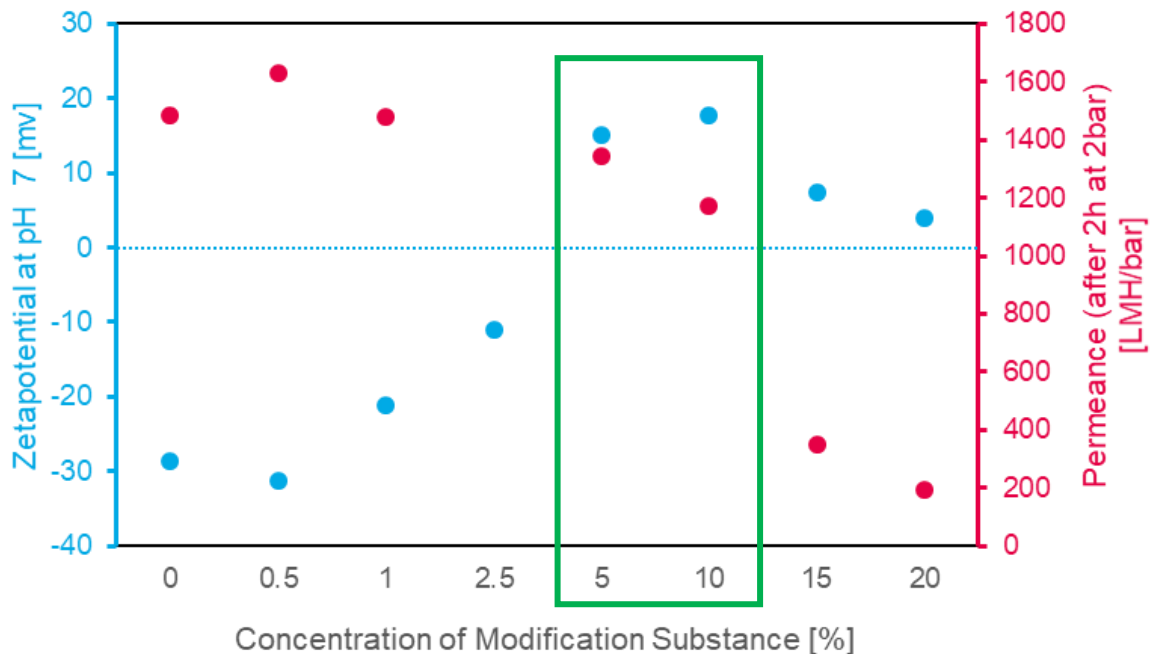
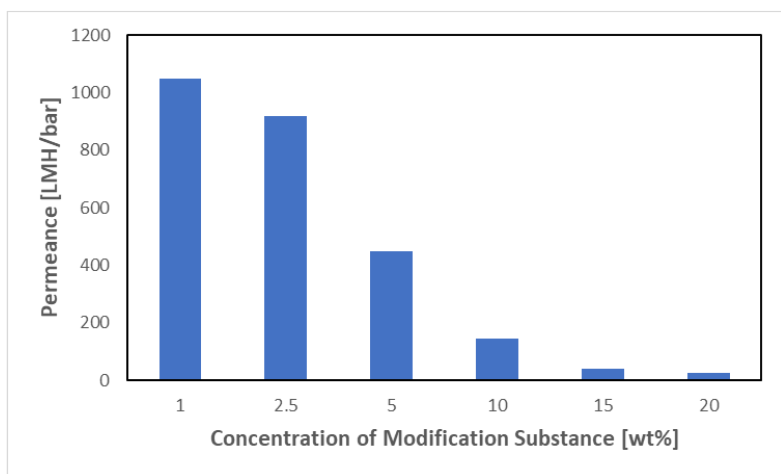
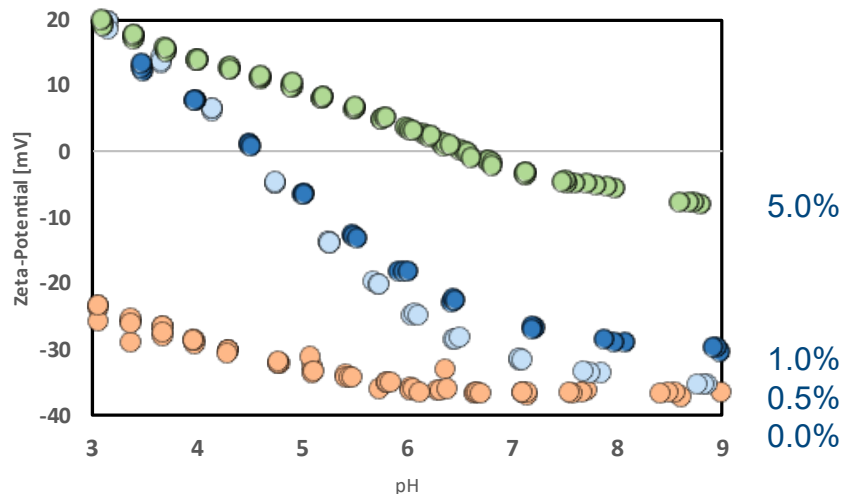
<https://uvebtech.com/articles/2015/modification-of-polymer-substrates-using-electron-beam-induced-graft-copolymerization/> (03.12.2020)

Modification strategy

Electron beam modification



Modification:

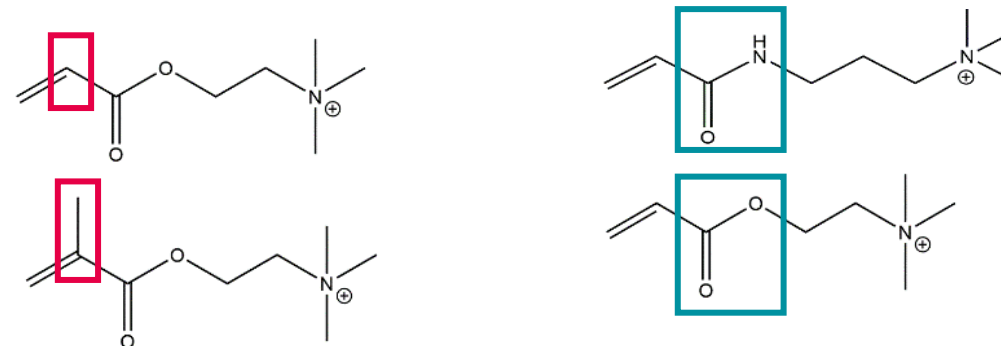
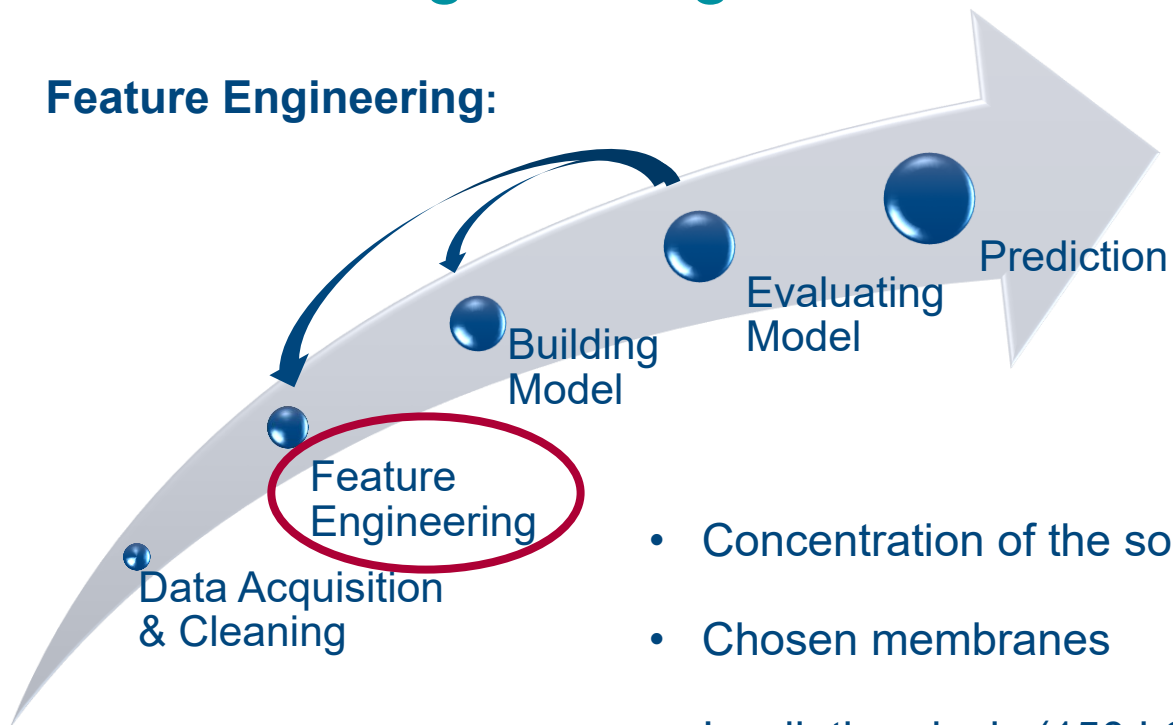


- Can we model/optimize the membrane modification?
- Can we predict new membrane modifications?

Application of Machine Learning Feature Engineering

* 0 = M2(sm. Pores), 1 = M1(big Pores)
+ quaternary amines = 14

Feature Engineering:

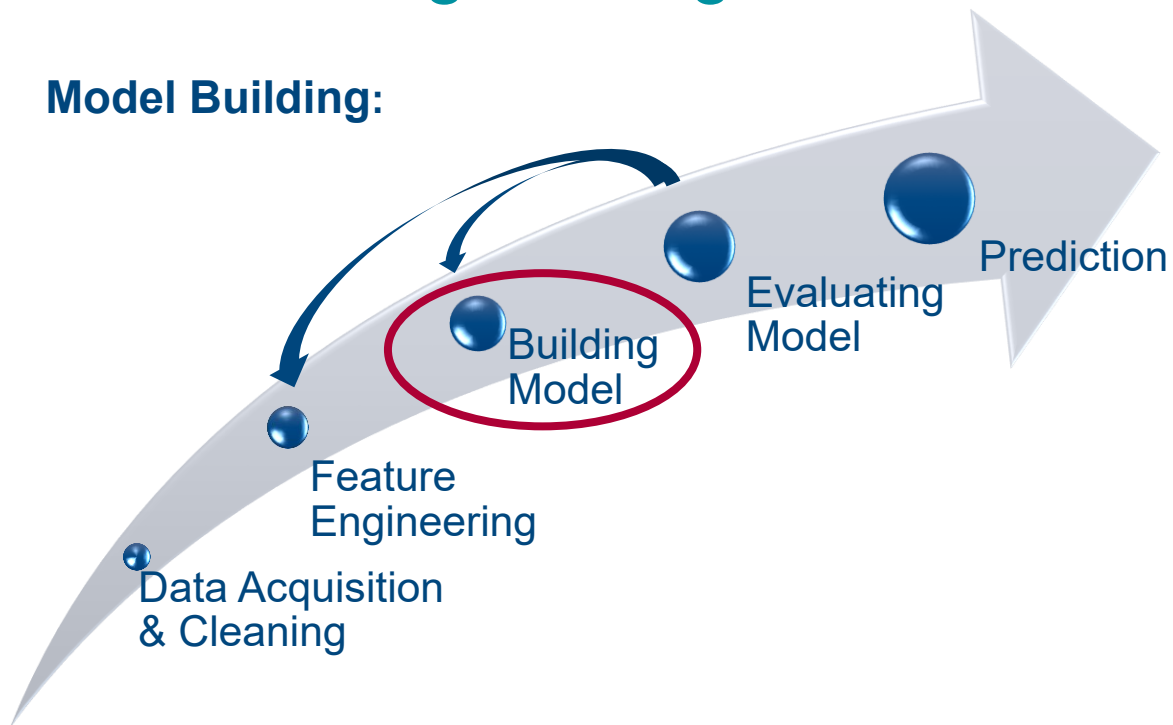


- Concentration of the solution (0.5-20 wt%) → • c [0.5...20]
- Chosen membranes → • Membrane [0; 1]*
- Irradiation dosis (150 kGy vs. 200 kGy) → • Dosis [150; 200]
- Modification substance → • pKa [0...14]⁺
- • Acryl [0; 1]
- • Methyl [0;1]

→ Each modified membrane gets a unique set of features to describe the modification

Application of Machine Learning Feature Engineering

Model Building:

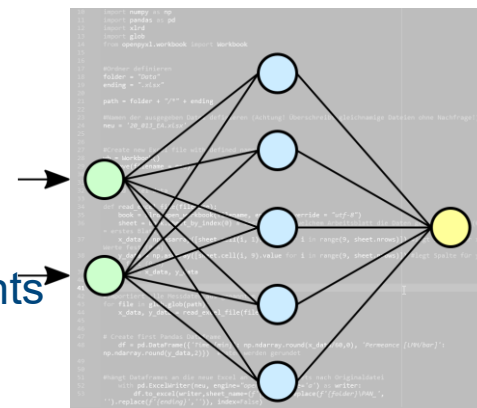


- Small amount of data (~50 unique membranes)

→ Ensemble Methods (Tree-based)

→ Artificial Neural Network

Input:
7/6 Features
42/51 Datapoints



Output:
Zeta-Potential
OR
Permeance

2 Hidden
Layers:

64 Neurons 16 Neurons

50 Epochs; upto 100 training cycles



Supervised Learning Approach:

- Each unique feature combination (membrane) is combined with a label/output value (zeta-potential/permeance)
- Possibility to extra-/interpolate
- Possibility to prediction new substances, if describable with features

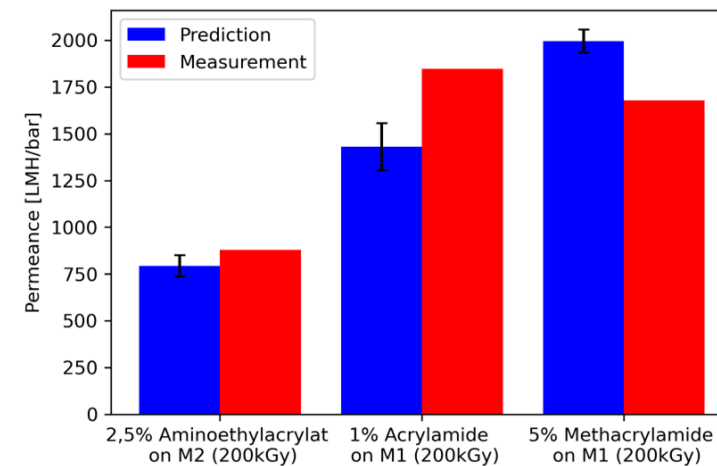
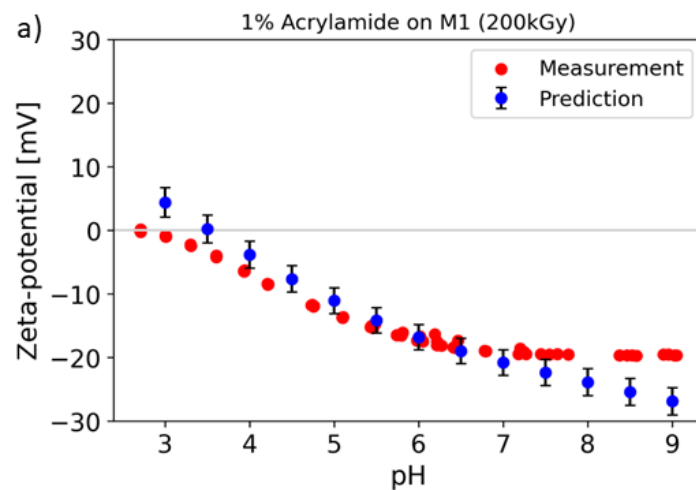
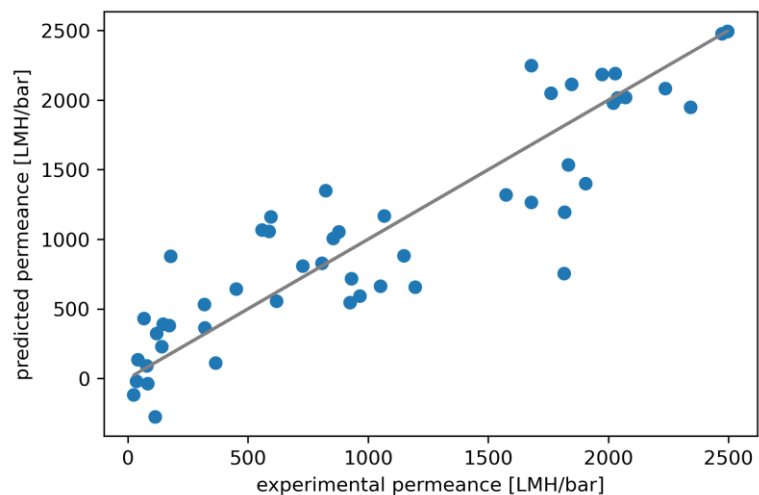
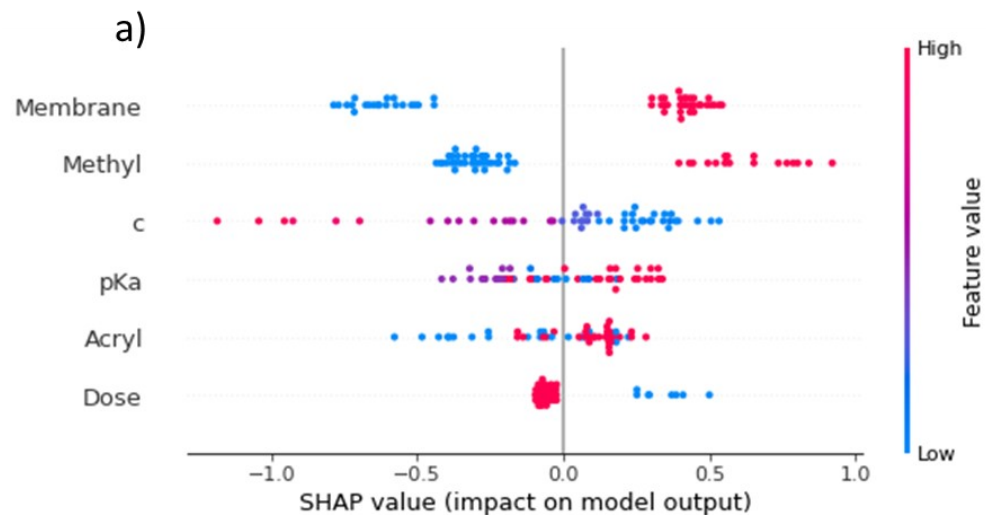


Application of Machine Learning

Prediction of New Membranes

Model Evaluation:

	R^2	Mean Absolute Error
Zeta Potential	0.968	1.6 mV
Permeance	0.984	105.9 LMH/bar

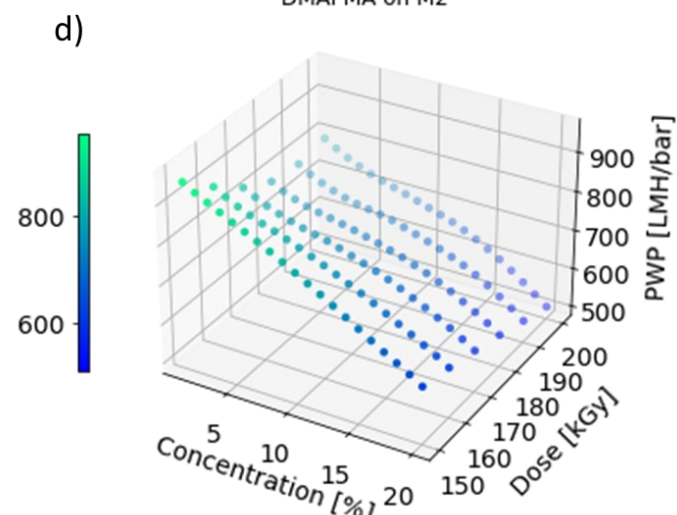
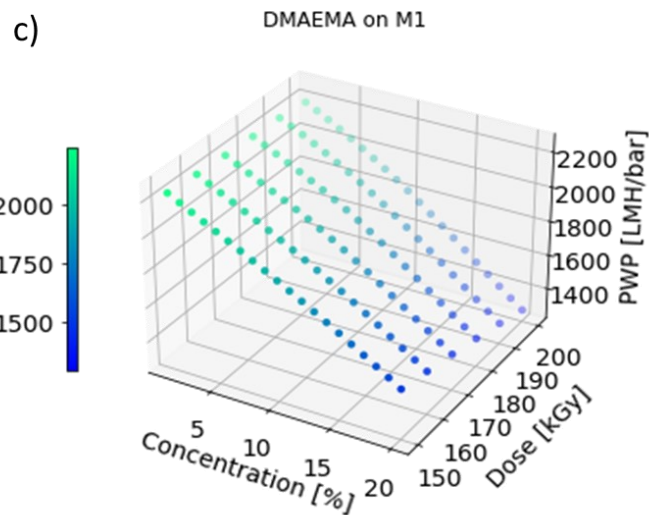
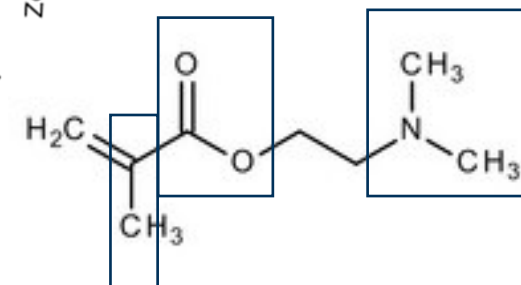
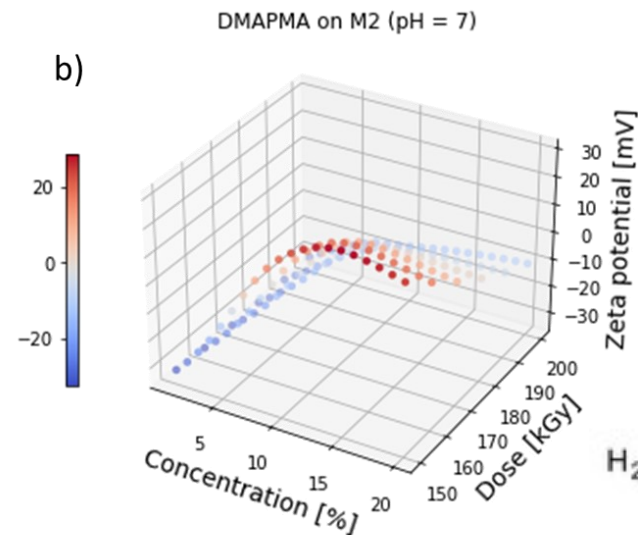
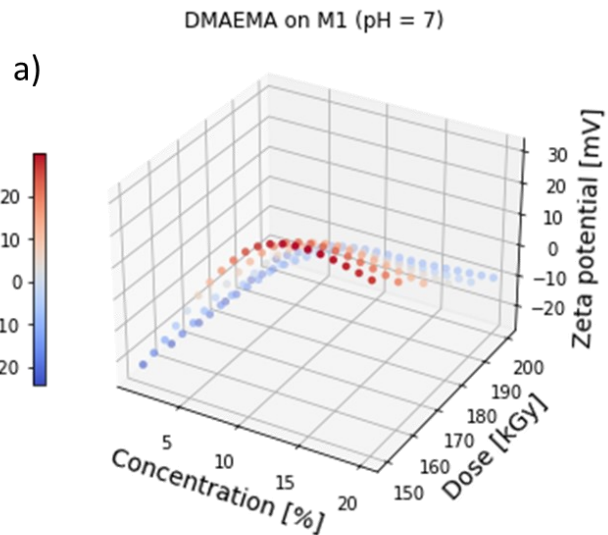
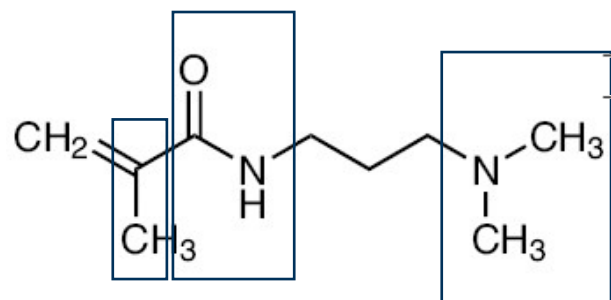


Application of Machine Learning

Prediction of New Membranes

*Mean value of 100 predictions per point

Prediction:

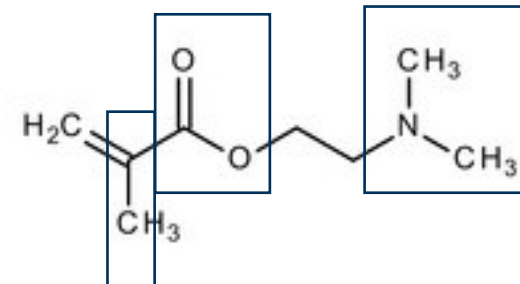


4 Membranes each were chosen, synthesised and analysed

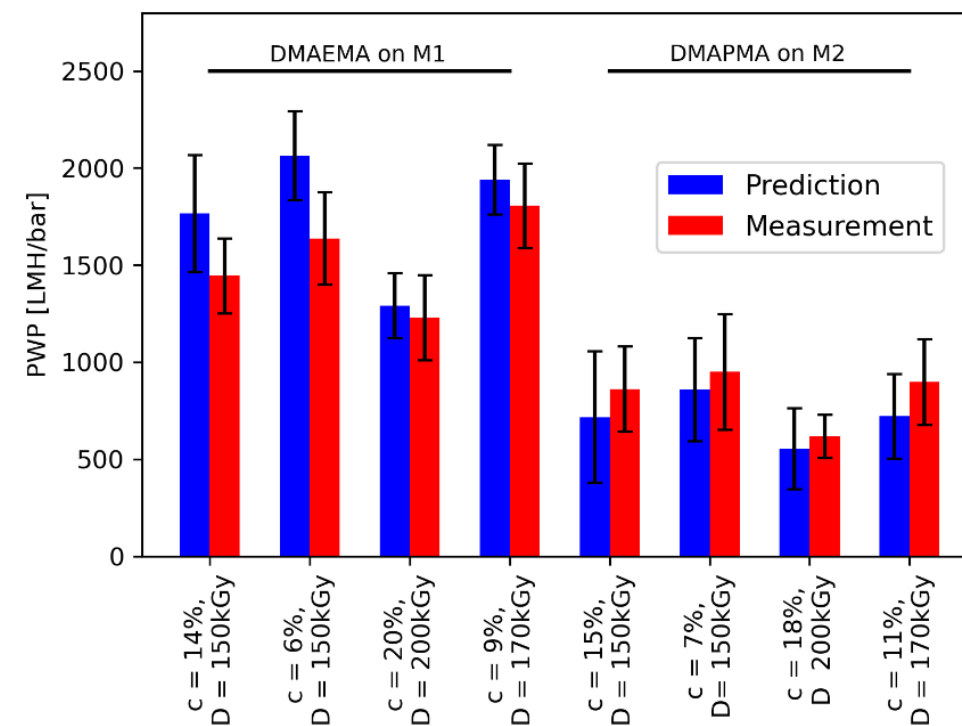
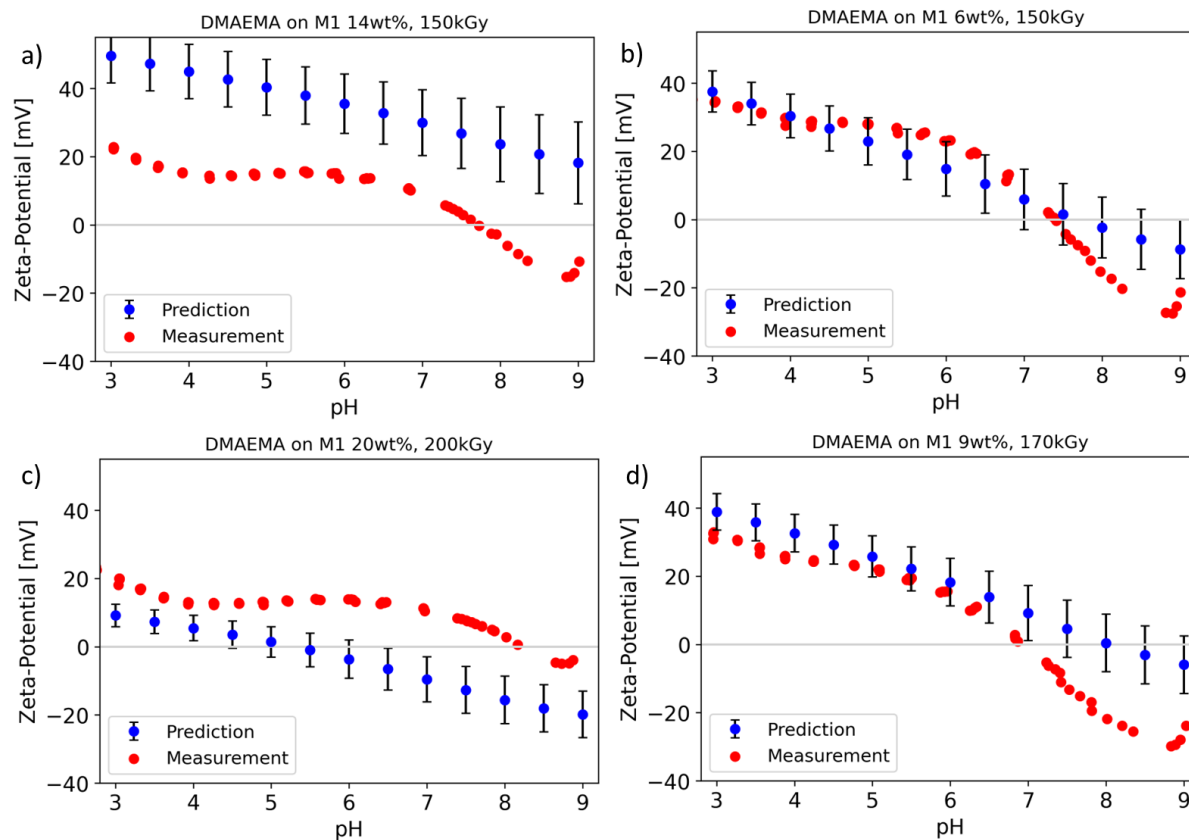
Computational time ~30 min (per output value)

Application of Machine Learning

Prediction of New Membranes



Can we predict new membrane modifications?



Outlook

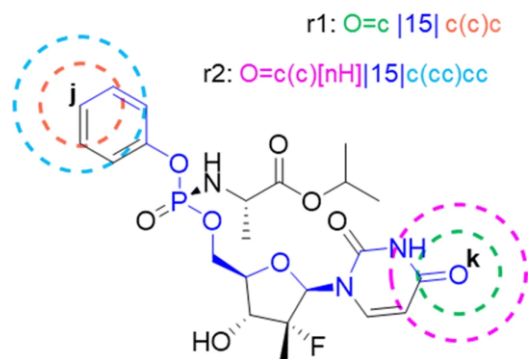
Generalization

Can we predict new membrane modifications?

- Modification substance

- pKa [0...14]⁺
- Acryl [0; 1]
- Methyl [0;1]

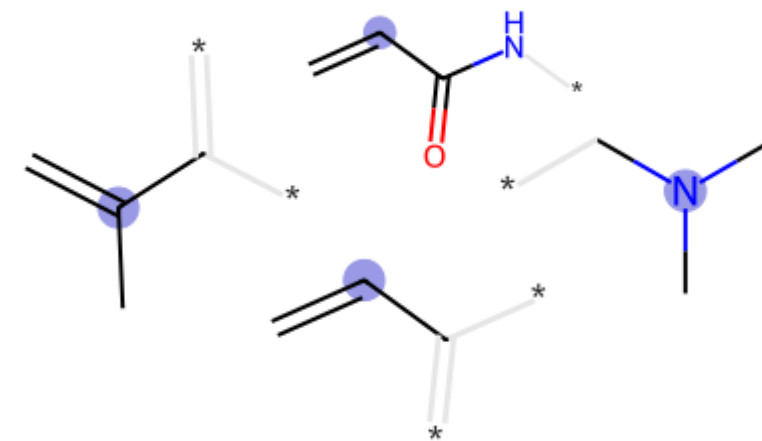
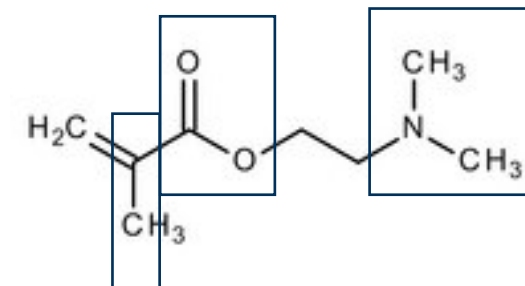
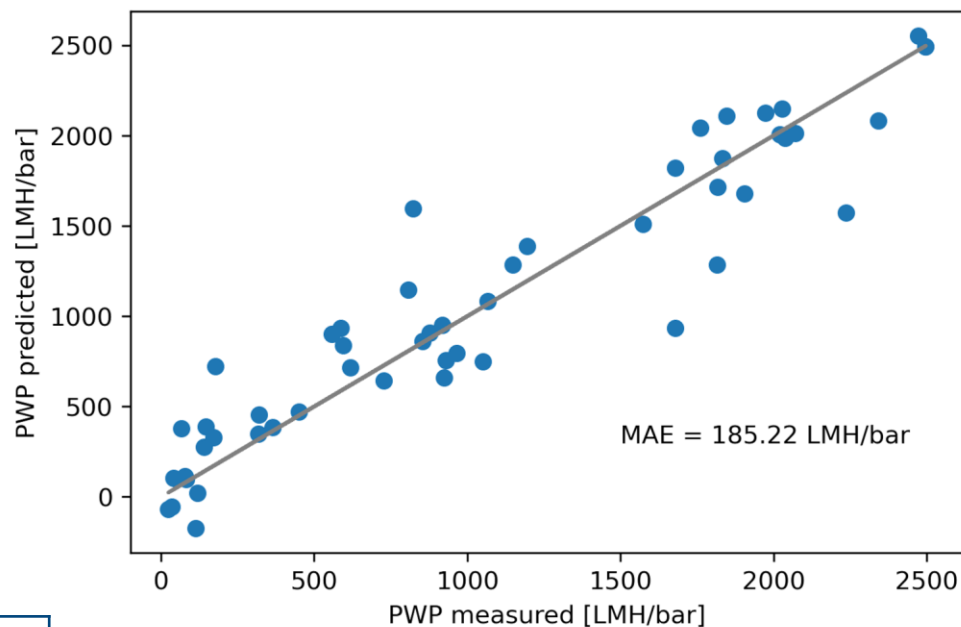
MAP4 encoding of jk



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1 0 1 1 0 0 0 0 1 0



→ Identify functional groups of importance

Summary

- Small and medium data sets can be applied in machine learning
- Regression models and neural networks showed high accuracy
- Low computational time
- New modification substances can be predicted
- Generalization possible

Acknowledgement

- Hereon-Institute of Membrane Research
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Thank you
for
your attention



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