TECHNISCHE UNIVERSITÄT DRESDEN

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Selektive Entfernung monovalenter Ionen aus salzhaltigen Wässern

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Bundesministerium für Bildung und Forschung

Institute of Urban and Industrial Water Management
Chair of Process Engineering in Hydro Systems

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MODELLING OF A SELECTIVE MEMBRANE CAPACITIVE DEIONIZATION PROCESS

D. Schödel, S. Tas-Köhler, K M N. Islam, H. Rosentreter, A. Lerch

MELPRO 2022, Praque, 19.09.2022

Presentation overview

1. Introduction to Membrane Capacitive Deionization technology
2. Goals of our innovatION project
3. Flow modeling
4. Electrochemical modeling

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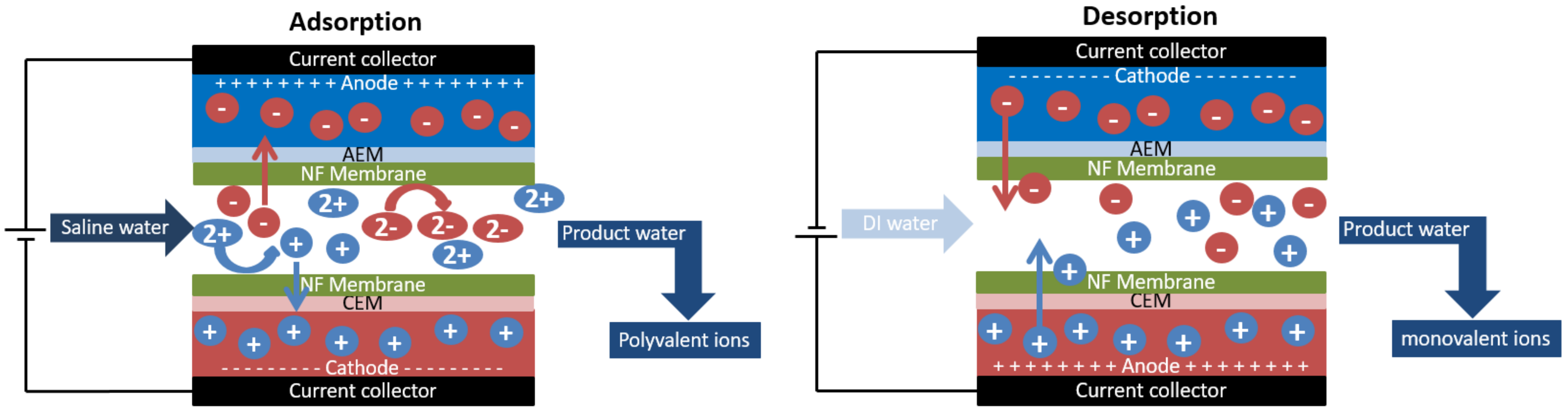
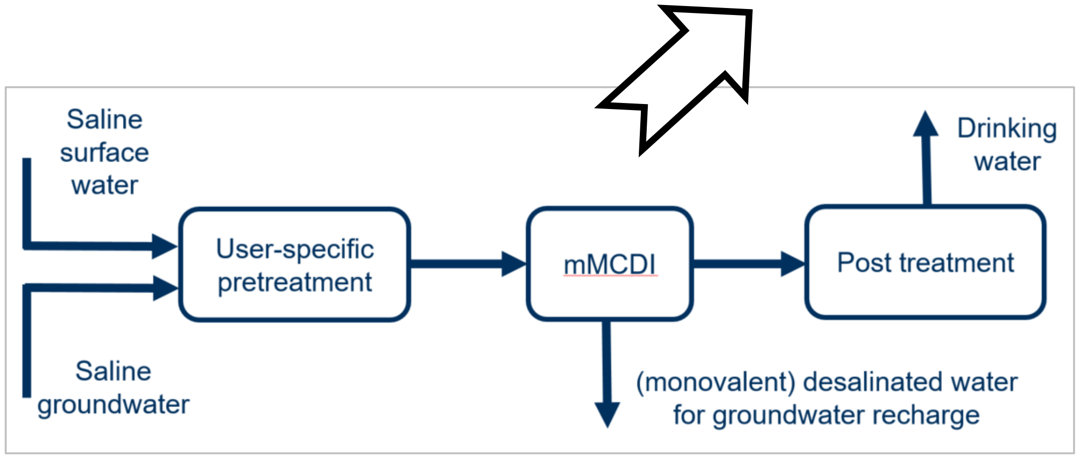
Membrane Capacitive Deionization (MCDI) Process



Principle of a monovalent selective MCDI with NF membranes



Process principle for implementation of mMCDI (monoselective membrane capacitive deionization) in desalination of saline waters

- Spacer filled flow channel
- Ion exchange membranes for ion retention during desorption
- Nanofiltration membranes to retain polyvalent ions (optional)
- Activated carbon electrodes

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... consists of 11 partners from science and industry:

Technische Universität Dresden
Carl von Ossietzky Universität Oldenburg
ipf Leibniz-Institut für Polymerforschung Dresden
fumatech Funktionelle Membranen und Anlagentechnologie BWT GROUP
elkoplan staiger GmbH Automation
DEUKUM
Kreisverband für Wasserwirtschaft WASSER
OOWV
KWR
United Nations University UNU-FLORES

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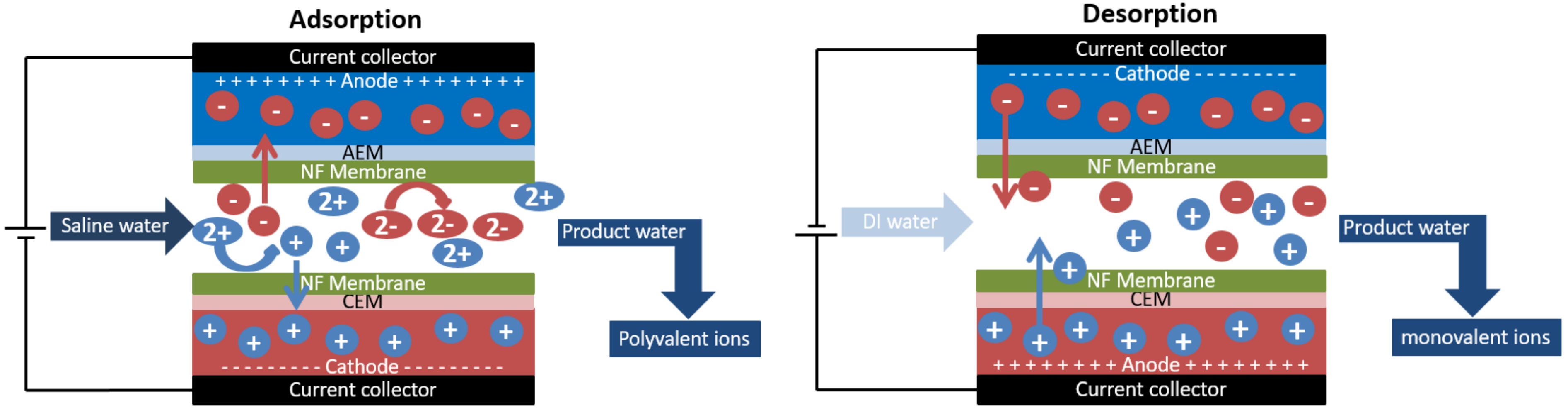
Membrane Capacitive Deionization (MCDI) Process



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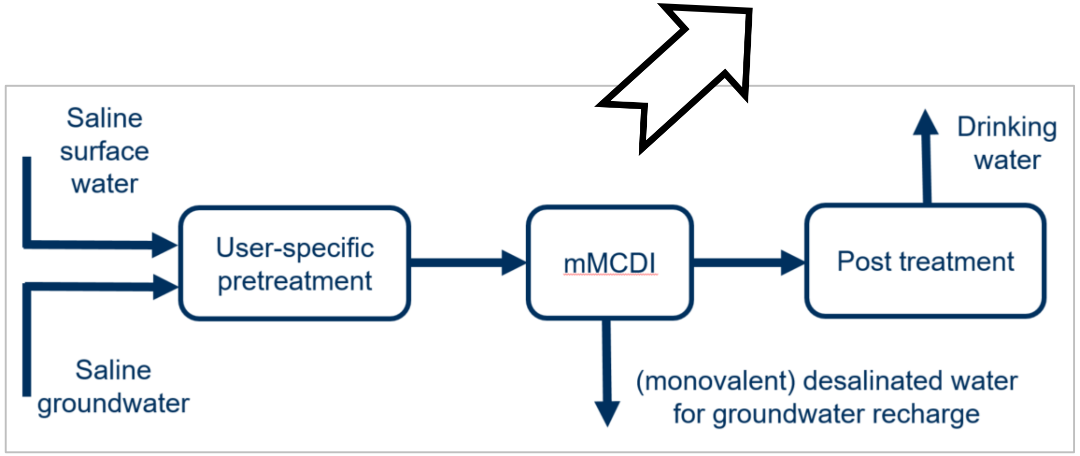

Process principle for implementation of mMCDI (monoselective membrane capacitive deionization) in desalination of saline waters

$$I_{el} = \frac{F \cdot Q_F \cdot \sum(c_{F,i} - c_D)}{\eta_I}$$

I_{el} – electrical current

F – Faraday's constant

η_I – current efficiency

c_D – aimed average diluate concentration

$c_{F,i}$ – feed concentration of ion I

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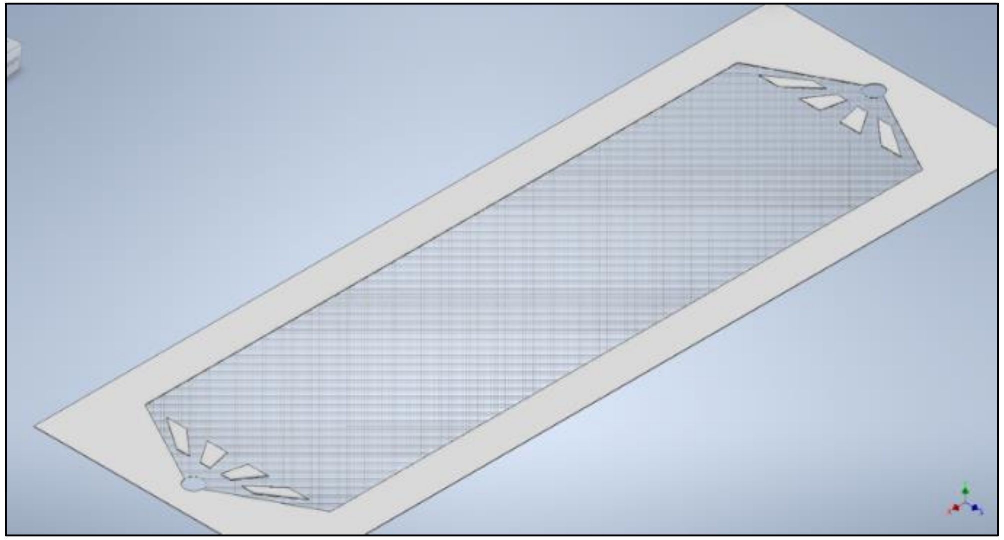
Modeling of a selective Membrane Capacitive Deionization Process

Flow model using ANSYS 2021R2

Goals:

- Geometry optimization in terms of pressure loss
- Optimizing flow distribution in stack arrangements



Spacer filled flow area (Franz, 2021)

Challenges:

- 270 and 500 µm Spacers fill flow channel, filament distance 0,83 and 1,67 mm respectively

  → Very detailed structure is substituted as porous media

- Very high length to height ratio can result in fine mesh

  → hybrid mesh with coarser mesh in middle area

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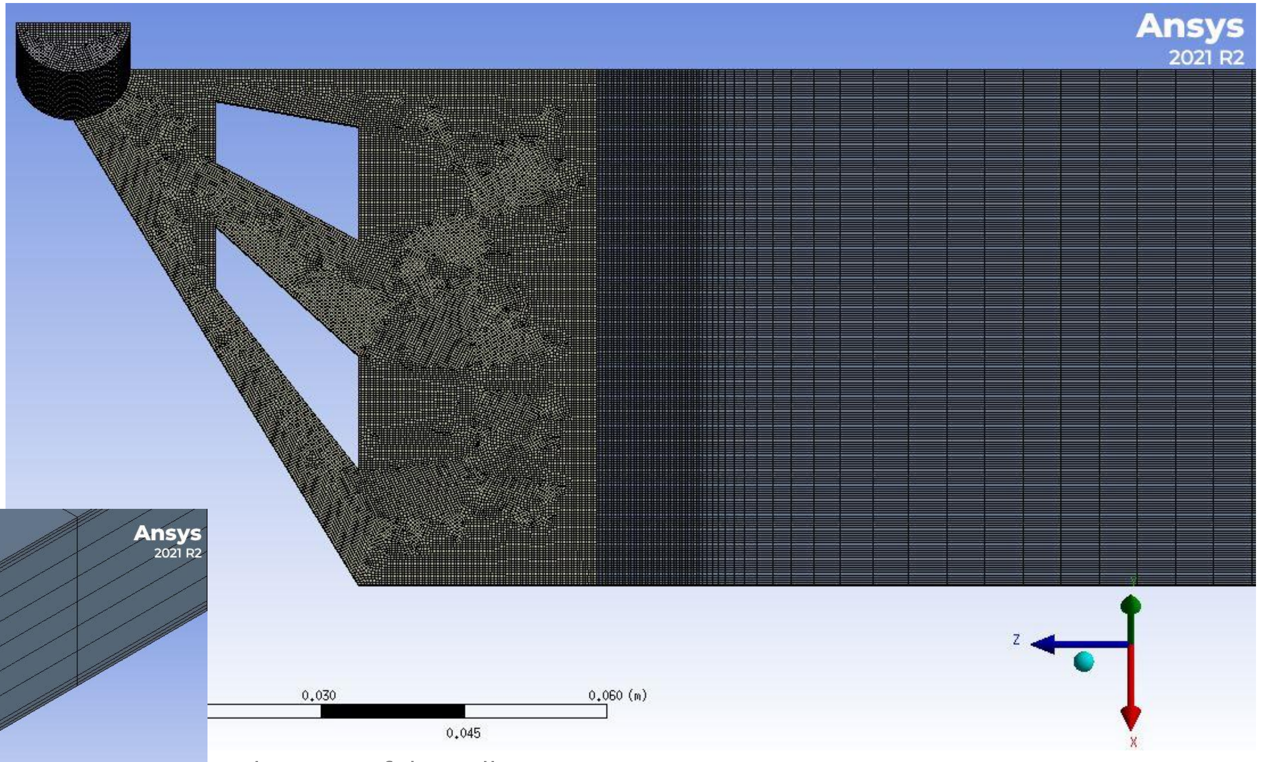
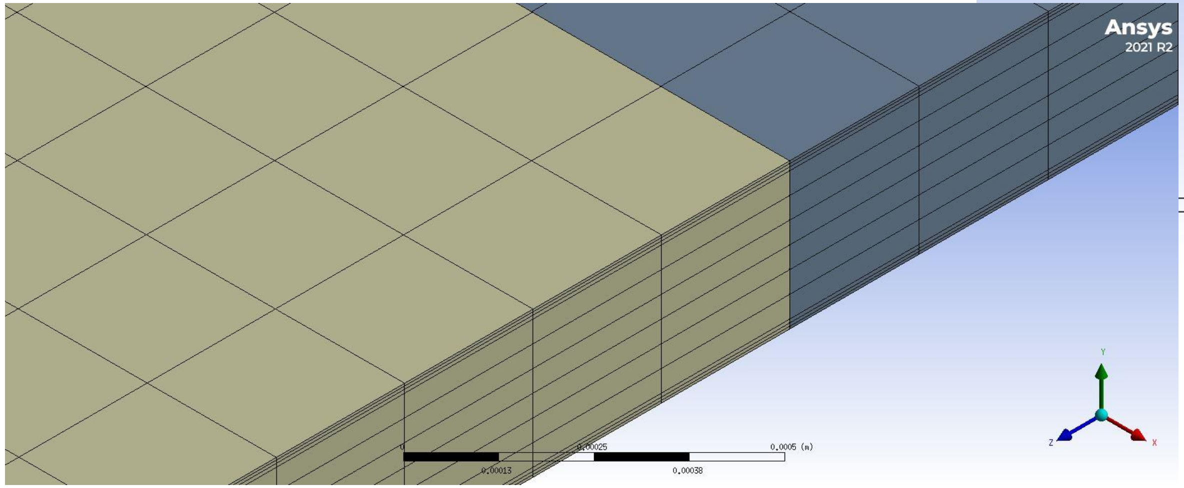
Structured mesh

- Symmetry in flow direction
- Structured mesh with coarser elements in geometrically uniform middle part



Inlet area of the cell



Contact region showing Inflation Layer and vertical divisions

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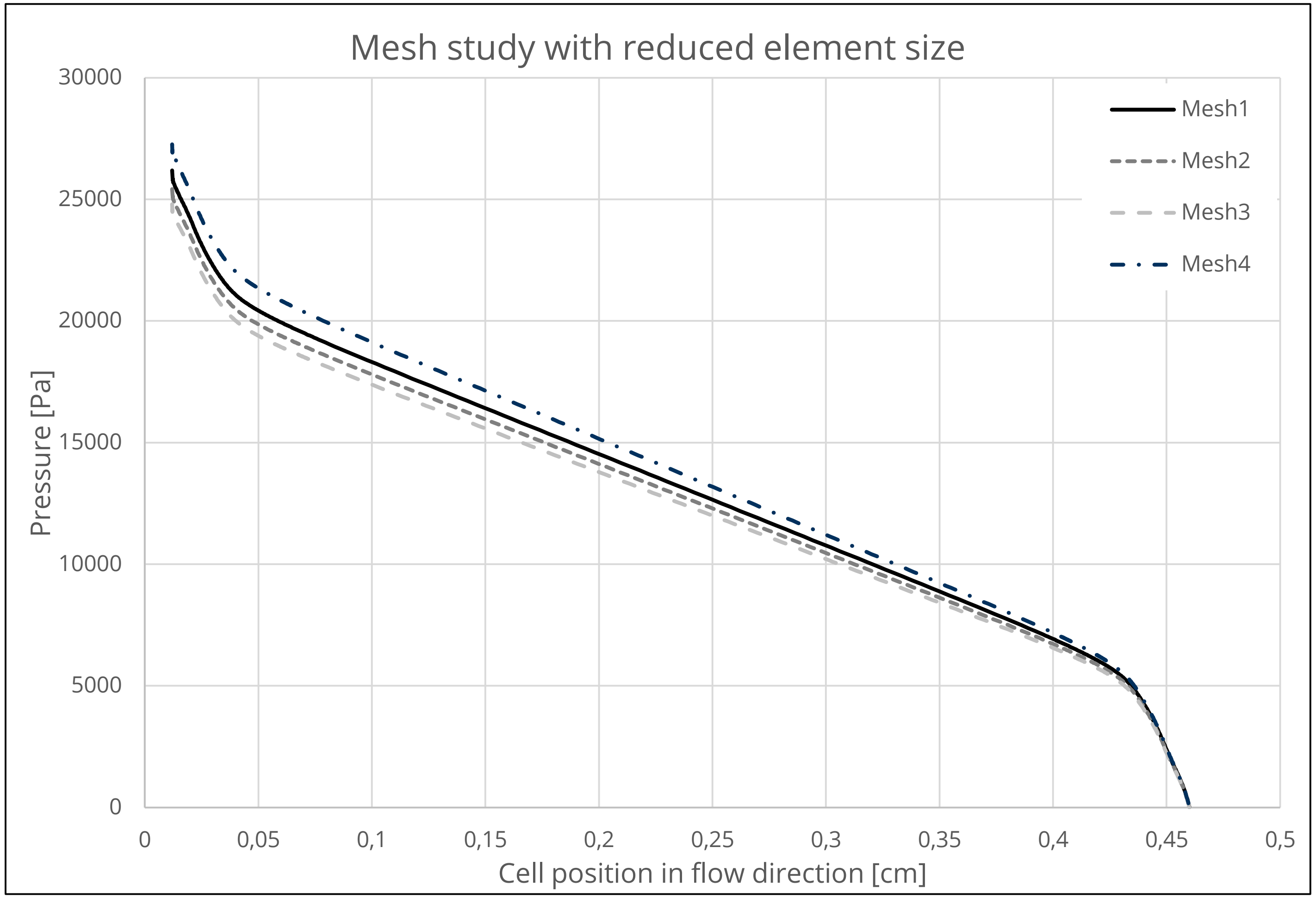
Mesh study

Solver settings:

- Second Order Equations
- Viscous Model: k-omega SST

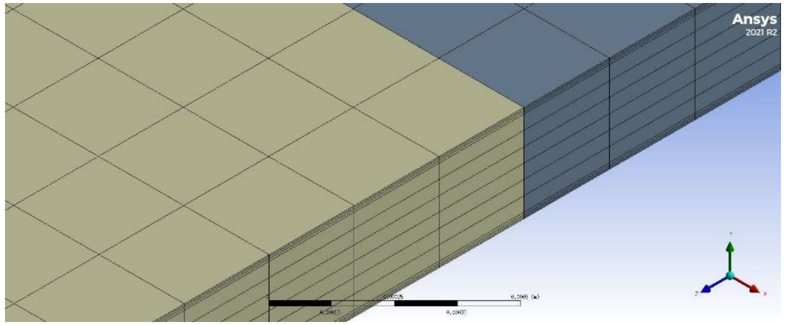
Mesh parameters

	mesh1	mesh2	mesh3	mesh4	mesh5
Mesh	4,00E-03	3,20E-03	2,56E-03	2,05E-03	1,64E-03
Body size	3,00E-04	2,40E-04	1,92E-04	1,54E-04	1,23E-04
Multizone spacer	2,70E-04	2,16E-04	1,73E-04	1,38E-04	1,11E-04
Multizone pipes	1,00E-02	8,00E-03	6,40E-03	5,12E-03	4,10E-03
Contact Sizing	3,00E-04	2,40E-04	1,92E-04	1,54E-04	1,23E-04
Contact Sizing 2	3,00E-04	2,40E-04	1,92E-04	1,54E-04	1,23E-04
Inflation	2,00E-05	1,60E-05	1,28E-05	1,02E-05	1,02E-05



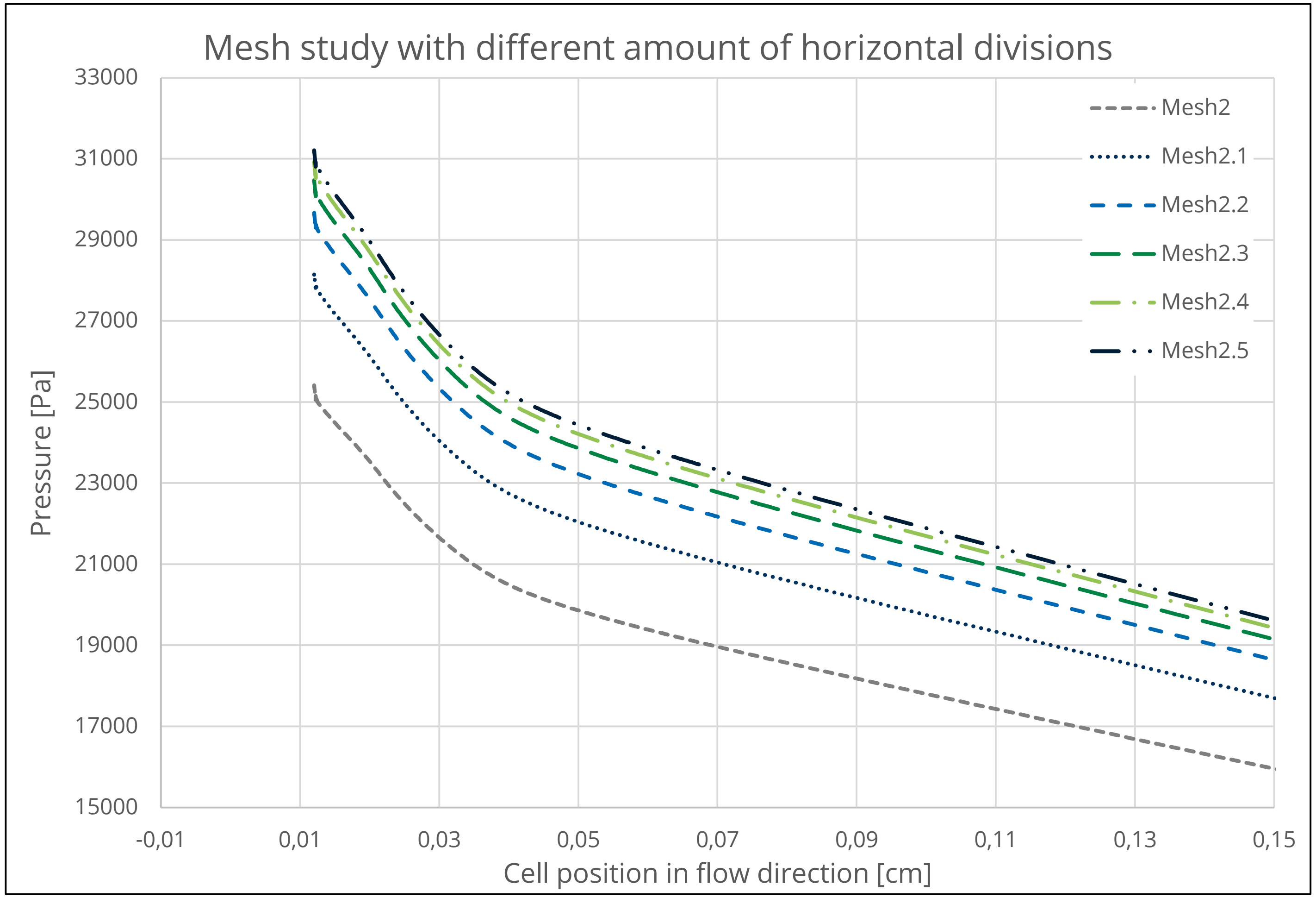
Pressure loss for different meshes

Mesh study



Mesh parameters

	mesh2.1	mesh2.2	mesh2.3	mesh2.4	mesh2.5
Mesh	3,20E-03	3,20E-03	3,20E-03	3,20E-03	3,20E-03
Body size	2,40E-04	2,40E-04	2,40E-04	2,40E-04	2,40E-04
Multizone spacer	2,16E-04	2,16E-04	2,16E-04	2,16E-04	2,16E-04
Multizone pipes	8,00E-03	8,00E-03	8,00E-03	8,00E-03	8,00E-03
Contact Sizing	2,40E-04	2,40E-04	2,40E-04	2,40E-04	2,40E-04
Contact Sizing 2	2,40E-04	2,40E-04	2,40E-04	2,40E-04	2,40E-04
Inflation	1,60E-05	1,60E-05	1,60E-05	1,60E-05	1,60E-05
Edge Sizing Divisions	2	3	4	6	7



Pressure loss for different meshes

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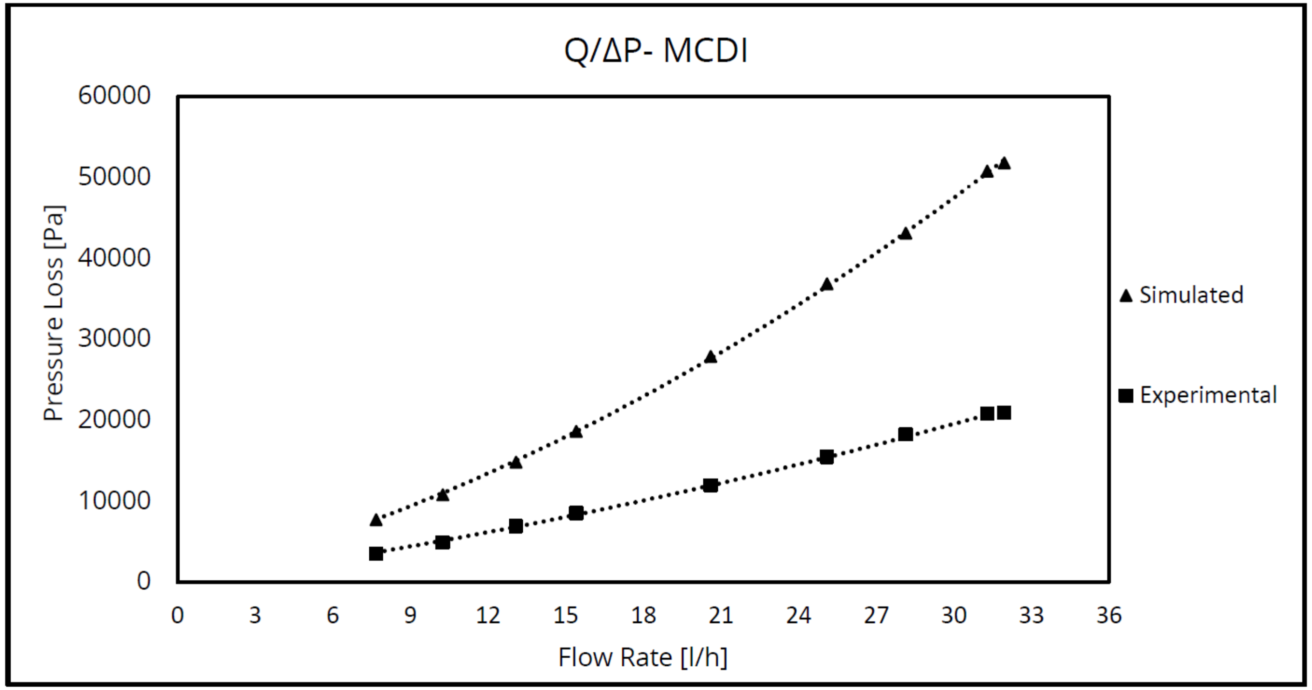
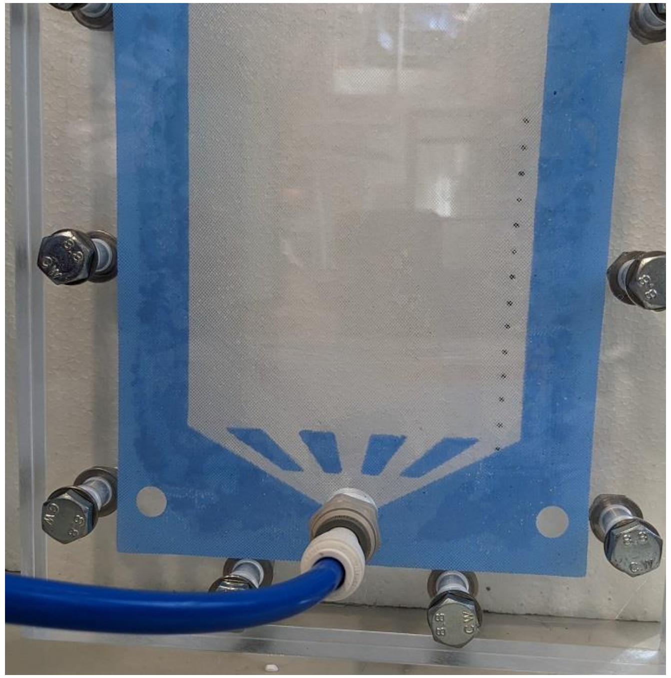
Model calibration and validation

- Input parameters (inertial and viscous resistance factors) are calculated from experimental results
- Pressure loss was determined by using a flow test cell



Comparison between simulated and experimental results (Islam, 2022)



Transparent flow test cell

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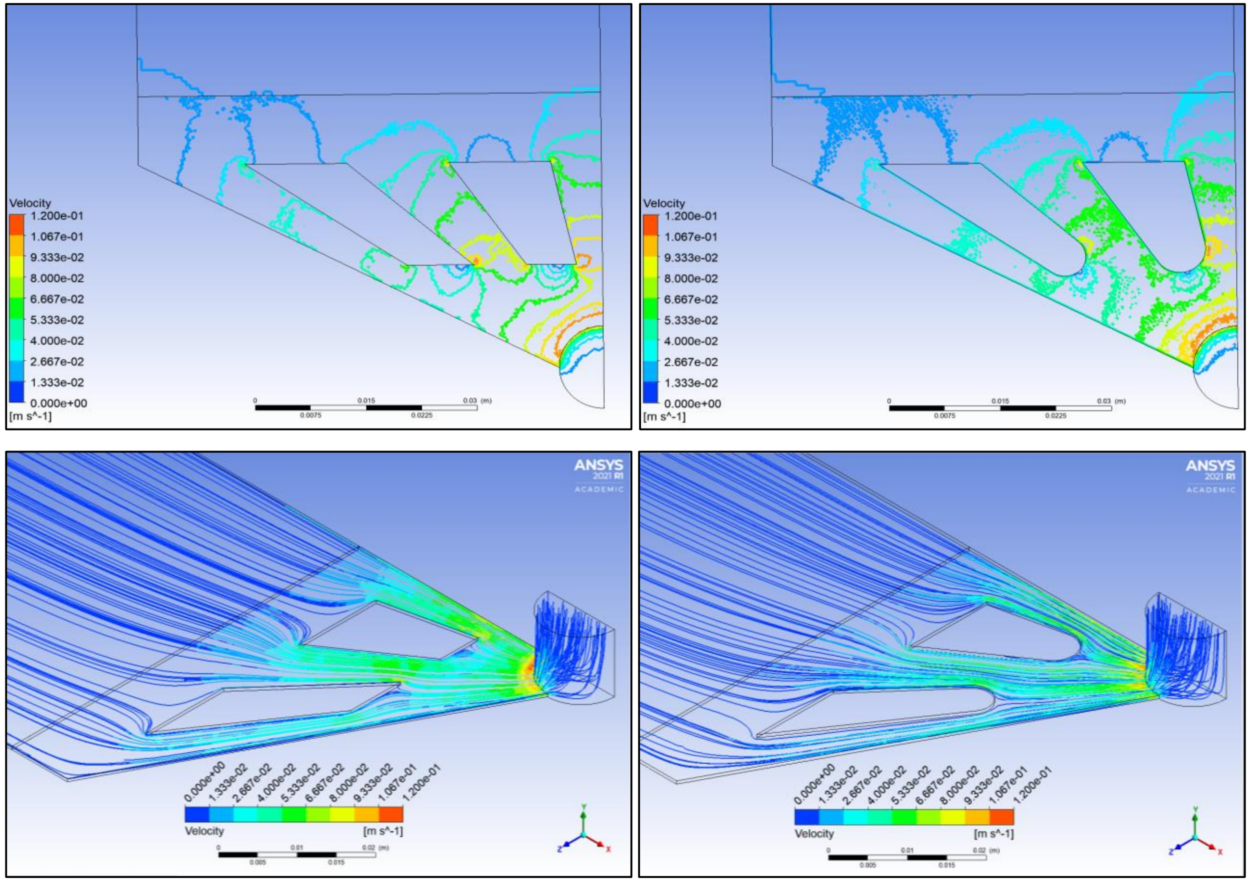
Geometry optimization

- Simulating different diffusor shapes with pressure loss reduction of > 20 %



Isotaches (top) and velocity track (bottom) for standard diffusor shape (left) and optimized geometry (right) (Franz, 2021)

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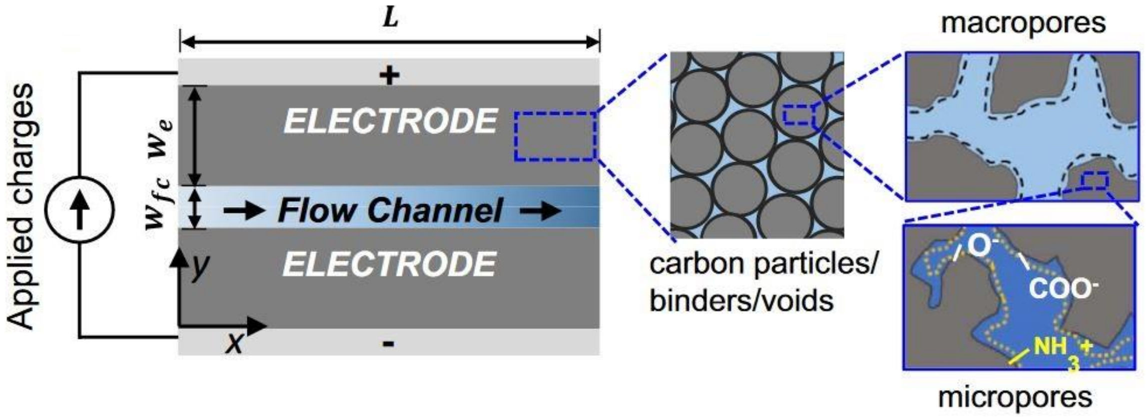
Electrochemical model on electrode scale

- Different materials are involved:
  - Electrodes are made from porous materials, therefore ion transport and interactions take place in micro- and macropores
  - Ion exchange membranes or other functional surfaces
- Electrical double layers (EDL) are forming at electrolyte – solid interfaces
  - Overall electroneutral, but contains positively and negatively charged regions



Porous electrode structure (Shang, 2017)

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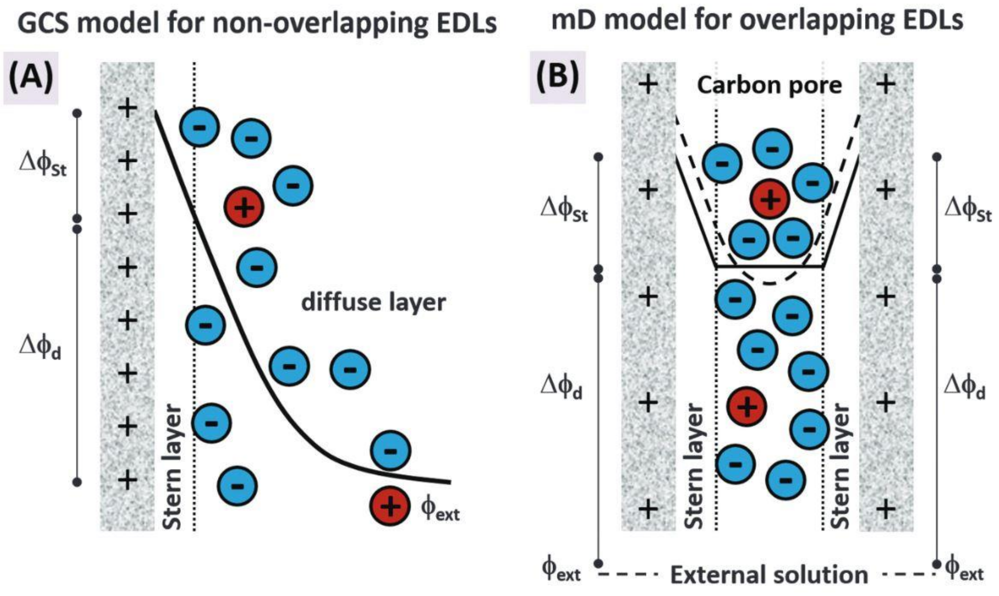
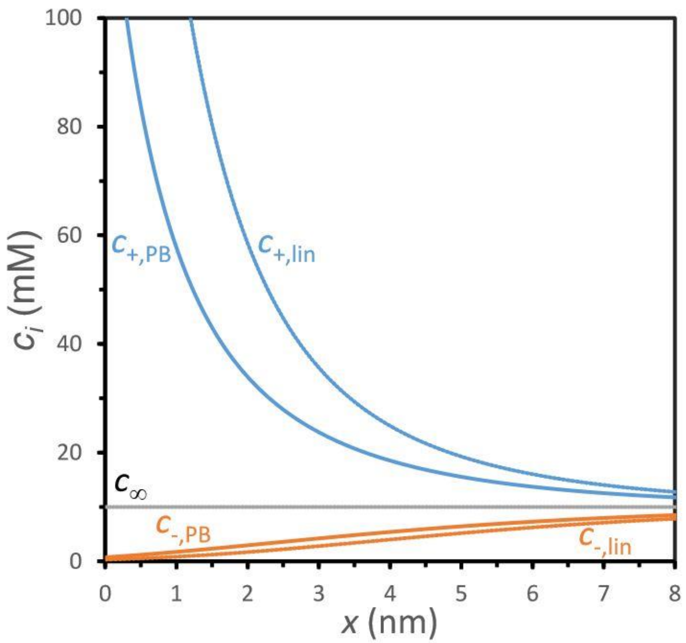
Electrical Double Layer

Several models to describe the Electrical Double Layer (Liu, 2020):

- Dynamic Langmuir theory
- Modified Donnan (mD)
- Gouy-Chapman-Stern (GCS)



Formation of non-overlapping EDLs and overlapping EDLs (Suss, 2015)



Ion concentration for GCS model (denoted by PB) and a linearized solution (Biesheuvel, 2020)

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Summary and outlook

Flow modelling:

- Mesh element divisions rectangular to flow direction have high impact on simulation results
- Computational effort can be reduced when using coarse mesh in uniform areas (~ 3x less elements)

Electrochemical model

- Deriving model for 100 % monovalent selective membranes

  → results in 1:1 salt solution (valence of ions) in electrode area

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Thank you for your attention!

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