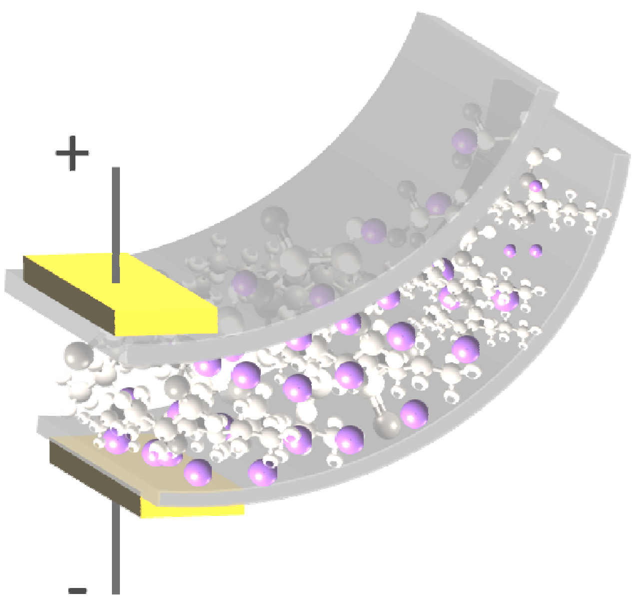
Smart Materials, Adaptive Structures & Intelligent Systems

September 21 – 23, Oxnard, California

Modeling IPMC material with dynamic surface characteristics



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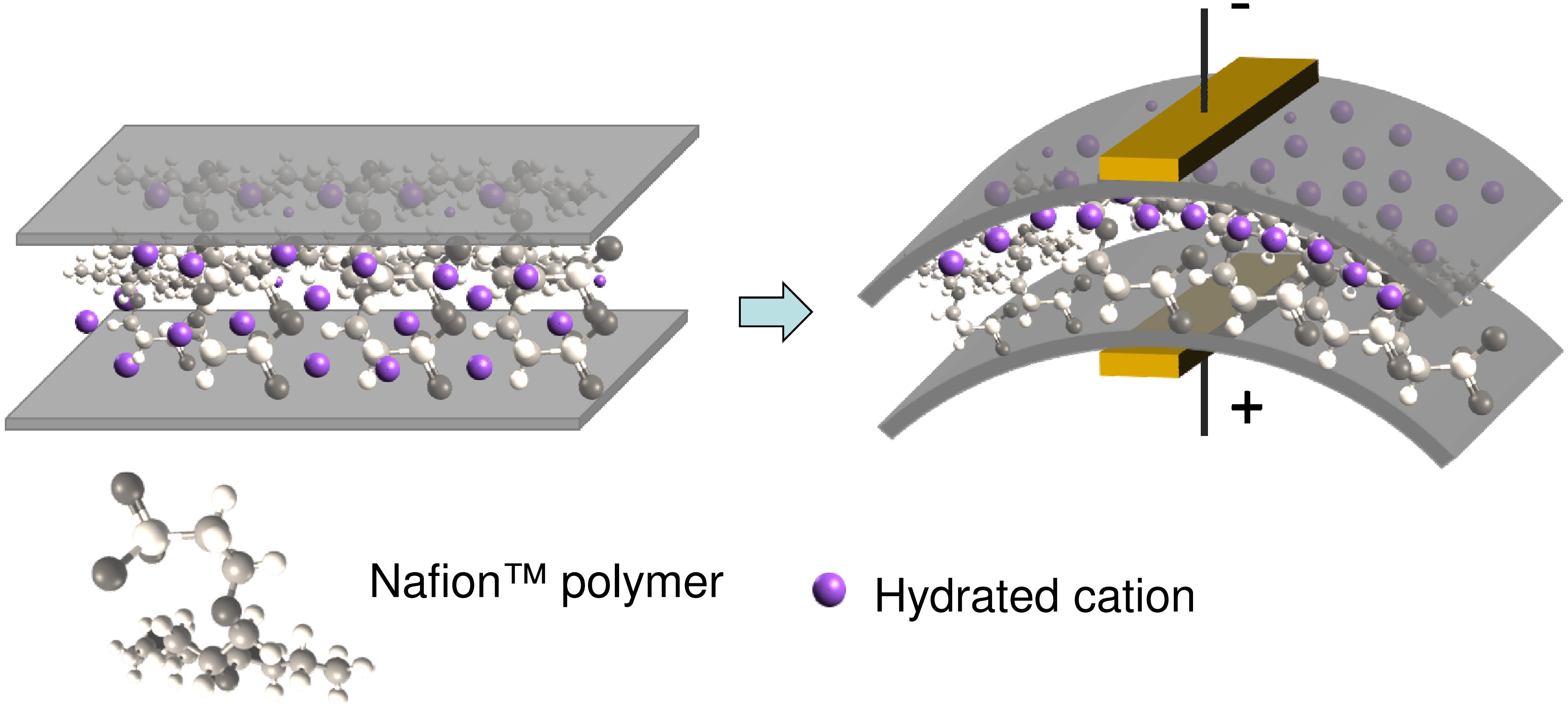
Outline

- IPMC material
- Basic mathematical description of the actuation
- Surface electrode model
  - Motivation
  - Physics background
  - Comsol Multiphysics simulations
  - Results
- Conclusions

IPMC material

- **IPMC – Ionic Polymer-Metal Composite**
  - **Electromechanical behavior**



  - **Mechanoelectrical behavior**

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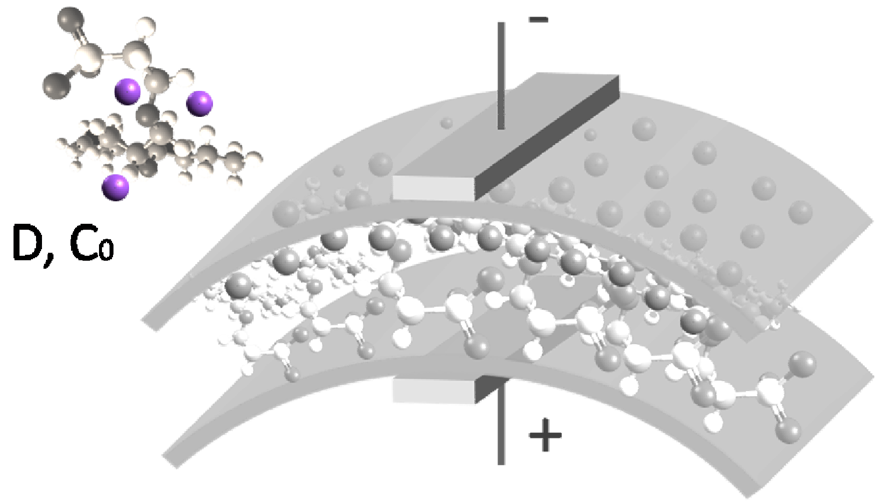
Simple model

- **The simple physical model:**
  - **Ion migration and diffusion, Nernst-Planck equation**

$$\frac{\partial C}{\partial t}+\nabla\cdot\left(-D\nabla C-z\mu FC\nabla\phi\right)=0$$

- C – cation concentration
- D – Diffusion coefficient
- z – charge number
- μ – mobility
- F – Faraday constant
- ϕ – electric potential



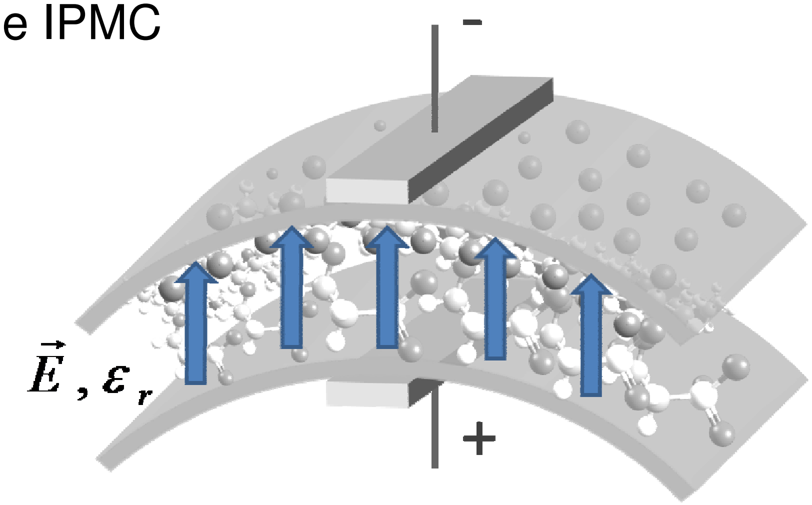
Simple model

- **The simple physical model:**
  - Ion migration and diffusion
  - **Electric field, Poisson' equation**

$$\frac{\partial C}{\partial t} + \nabla \cdot \left(-D \nabla C - z \mu F C \nabla \phi \right) = 0$$

$$\nabla \cdot \vec{E} = -\Delta \phi = \frac{F\rho}{\varepsilon}$$

- Describes the electric field in the IPMC
- E – electric field
- ϕ – potential
- ρ – charge density
- ε – electric permittivity
- F – Faraday constant

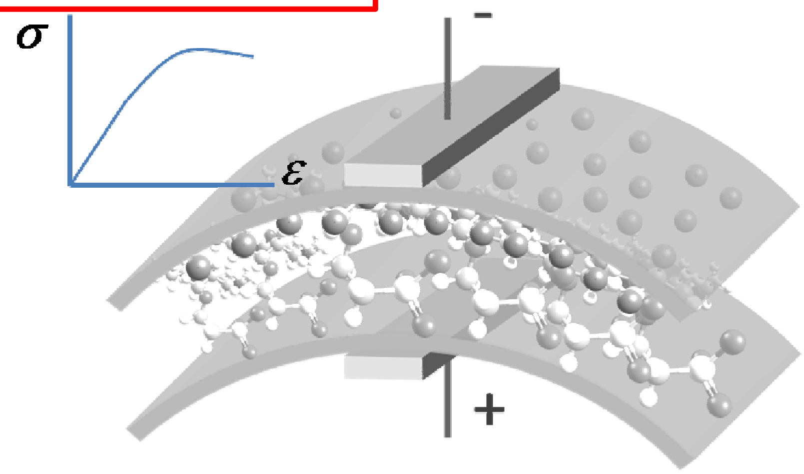


Simple model

- **The simple physical model:**
  - Ion migration and diffusion $\frac{\partial C}{\partial t} + \nabla \cdot \left(-D\nabla C - z\mu FC\nabla\phi \right) = 0$
  - Electric field, Poisson' equation $\nabla \cdot \vec{E} = -\Delta\phi = \frac{F\rho}{\varepsilon}$
  - **Stress-strain**

$$-\nabla \cdot \sigma = \vec{F}(\rho)$$

$$\sigma = D\varepsilon$$

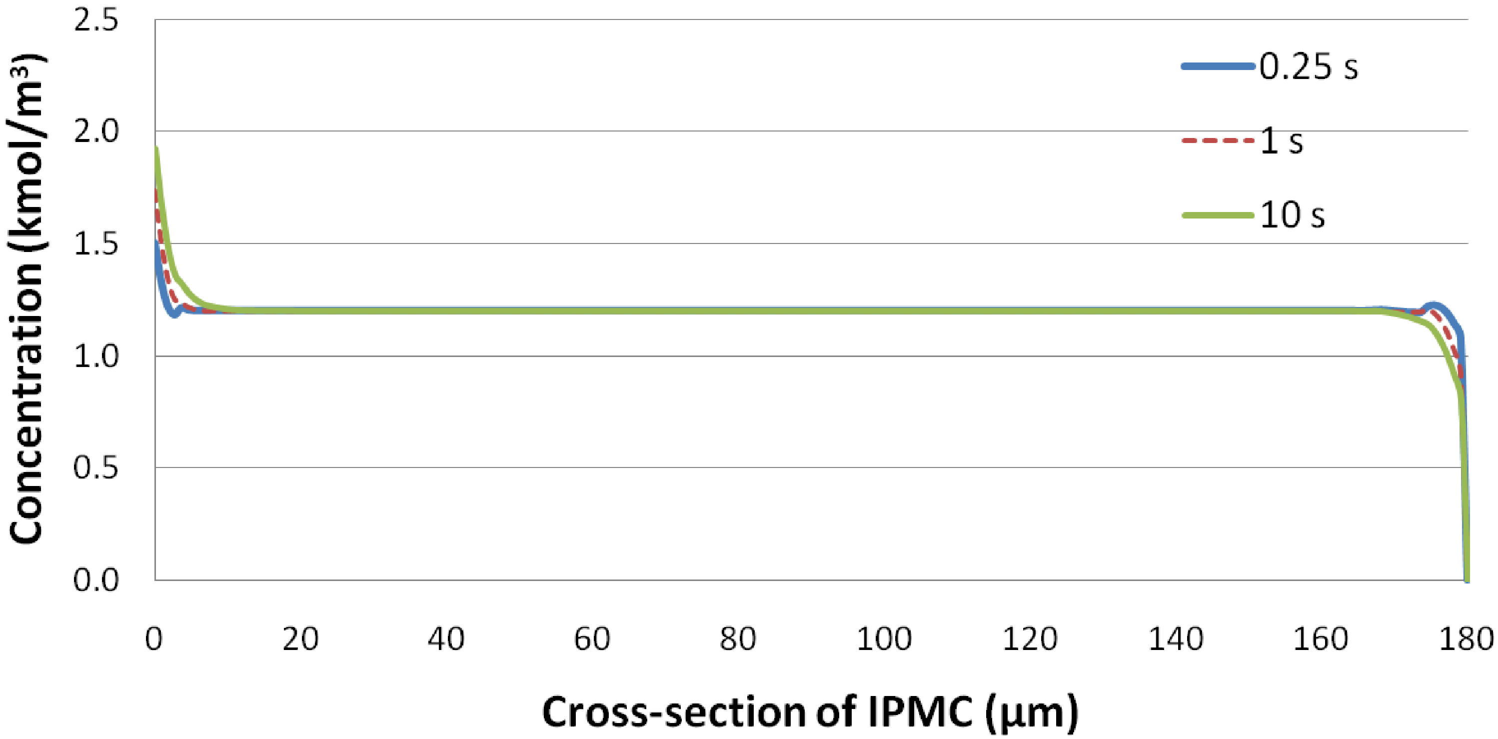


    - Stress is related to the charge density

  - **Not considered in this work**

Concentration - Bending

- **Concentration graph**

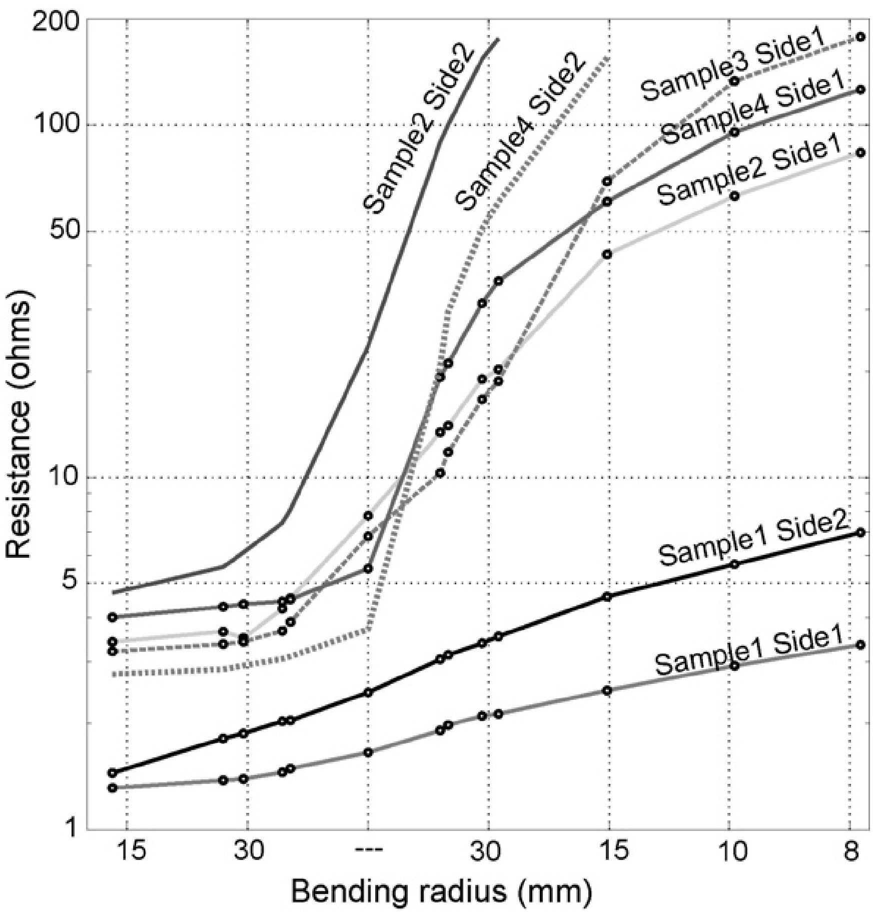


  - **Bending related to concentration → electric properties**

Electrode modeling - Motivation

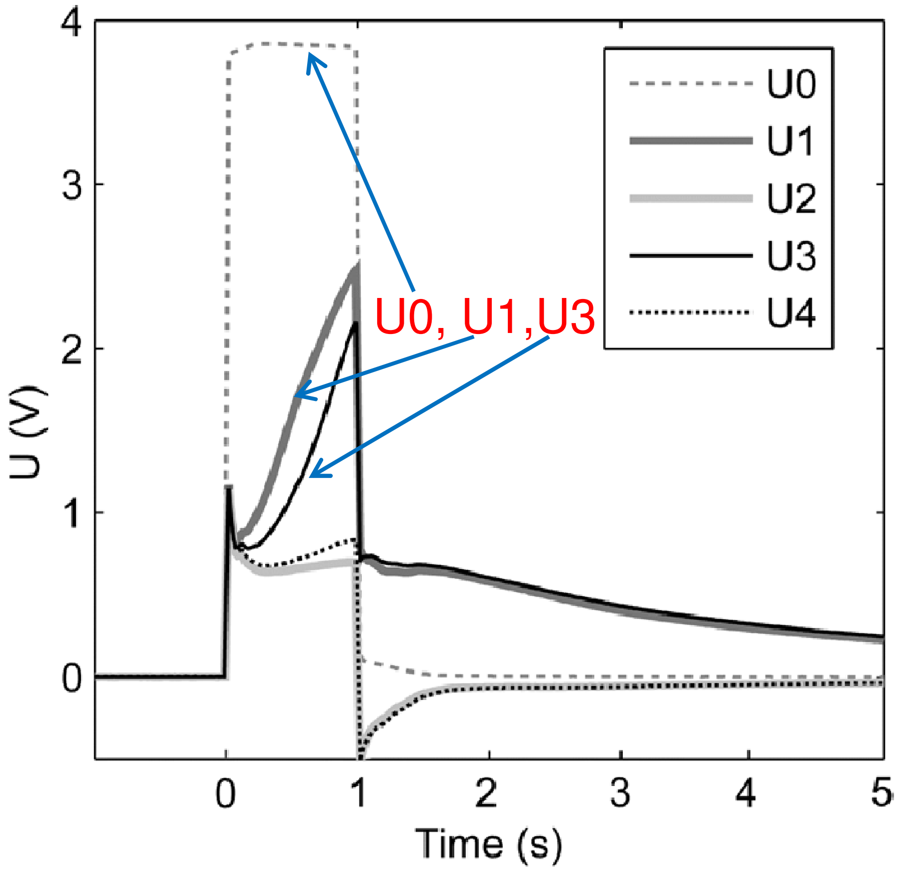
- **Modeling the effect of the electrodes on the potential inside the polymer. Why?**

  1)Some samples have shown significant dynamic surface resistance…



A. Punning, M. Kruusmaa and A. Aabloo, Sensors and Actuators, A: Physical **133** (1), 200 (2007).

Electrode modeling - Motivation



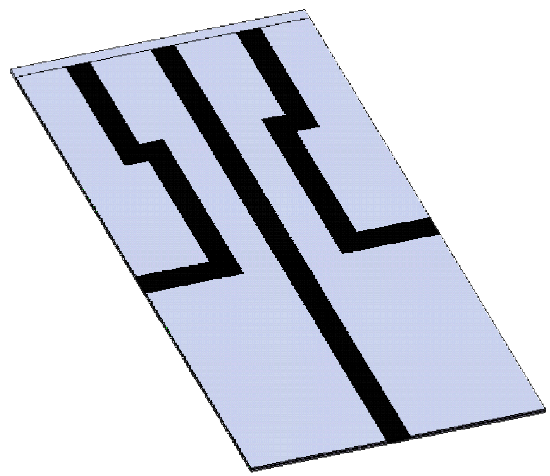
A. Punning, Dissertation Thesis, Tartu University, 2007.

- … which leads to a voltage drop along the electrode
  - U0, U1, U3 measured on the one side of IPMC
  - Some of the drop is due to electrolysis
  - Part of it is due to surface resistance

Electrode modeling - motivation

2) Patterned electrodes

- 3D bending
- Different areas with different surface characteristics

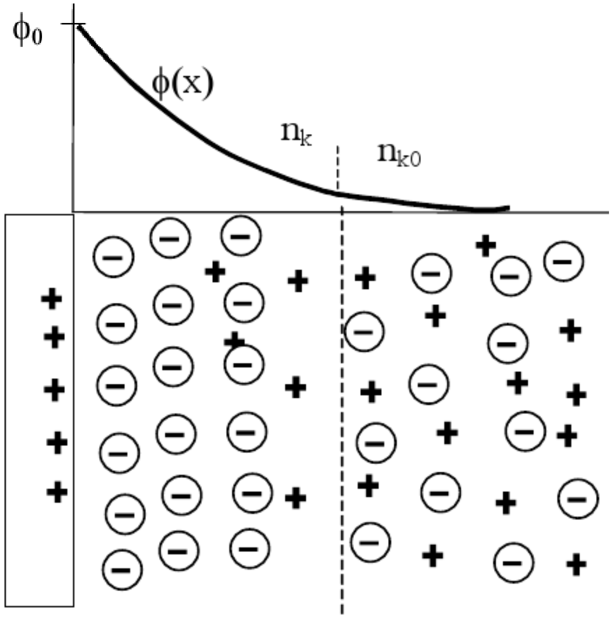


3) Electrode conductivity characterization

Surface resistance model - background

- **Tie together the current flowing through the surface and the ionic current inside the polymer**
- **Ramo-Shockley theorem**
  - **Plasma phycis ***
  - **Ion channels in proteins #**

Courtesy of M. Dingemans



Courtesy of M. Laan

* P. Paris, M. Aints, M. Laan, and T. Plank, “Laser-induced current in air gap at atmospheric pressure,” Journal of Physics D: Applied Physics 38(21), pp. 3900–3906, 2005.

W. Nonner, A. Peyser, D. Gillespie, and B. Eisenberg, “Relating Microscopic Charge Movement to Macroscopic Currents: The Ramo-Shockley Theorem Applied to Ion Channels,” Biophysical Journal 87(6), pp. 3716–3722, 2004.

Surface resistance model – math.

- **Current in the external circuit:**

$$I = \frac{1}{1V}\sum_j q_j \vec{W}(\vec{r}) \cdot \vec{v}_j$$

- **By integrating over arbitrary trajectories, the charge:**

$$Q = -\frac{1}{1V}\sum_j q_j \left[U\left(\vec{r}''_j\right) - U\left(\vec{r}'_j\right)\right]$$

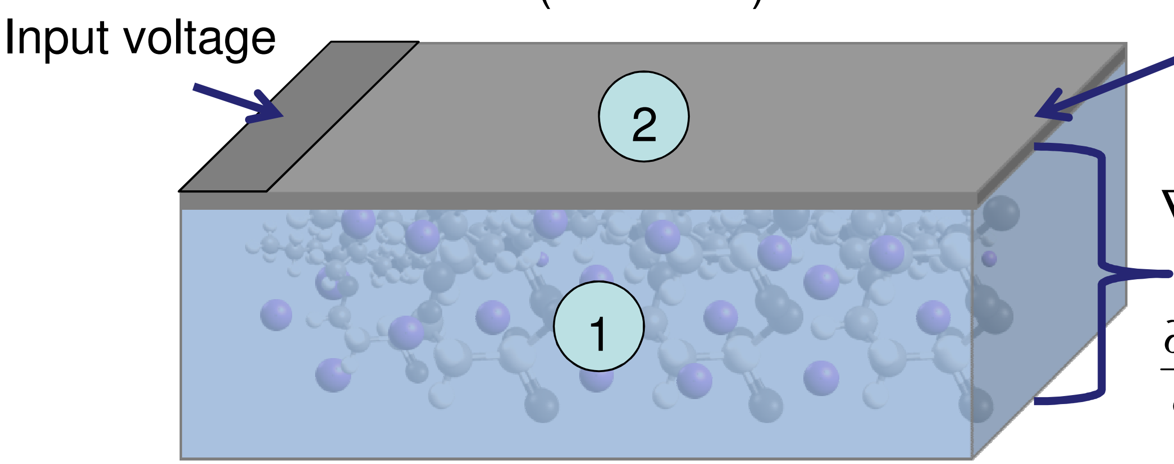
- **The following relation for current density can be derived:**

$$\vec{J} = \frac{F}{d}\int_0^d \vec{f} \cdot \vec{d}y \longleftarrow$$

Final form that is used in the simulations

Surface resistance model - Comsol

- **Implementation in Comsol**
  - **2 different domains are modeled**
    - 1: Polymer (Nernst-Planck and Poisson' equation)
    - 2: Electrode (Ohm' law)



$$\sigma \nabla V = \vec{j}$$

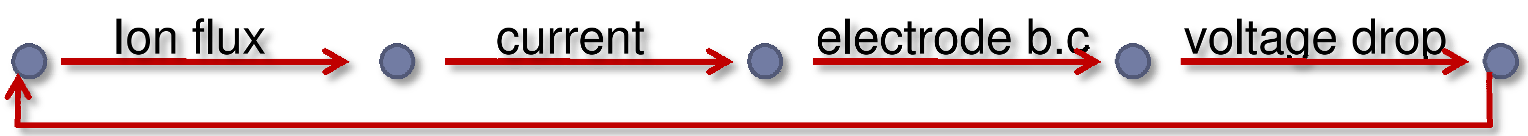
$$\nabla \cdot \vec{E} = -\Delta \phi = \frac{F\rho}{\varepsilon}$$

$$\frac{\partial C}{\partial t} + \nabla \cdot \left(-D \nabla C - z \mu F C \nabla \phi \right) = 0$$

  - **B.C. Boundary between the bulk Nafion and electrode:**
    - Integrated ion flux from domain 1 was projected as an input on domain 2: $\vec{j} = \frac{F}{d} \int_0^d \vec{f} \cdot \vec{d}y$

Surface resistance model - Comsol

- **The electric current inside the IPMC is calculated by integrating the ion flux**
- **The ion flux is “projected to the electrode” where it becomes a boundary condition for the electrode model**

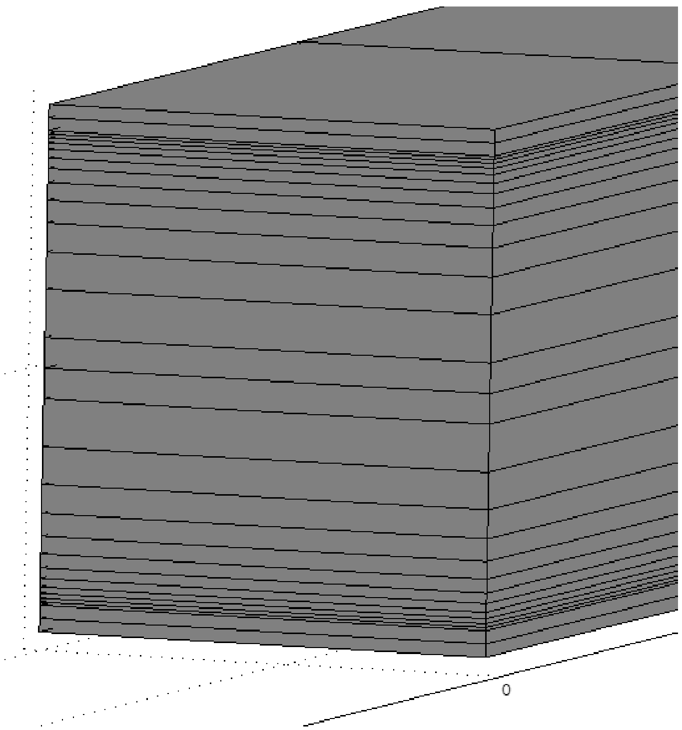


- **The voltage of the electrode model, in turn, becomes a boundary condition to the Poisson equation, which is responsible for the ion flux**

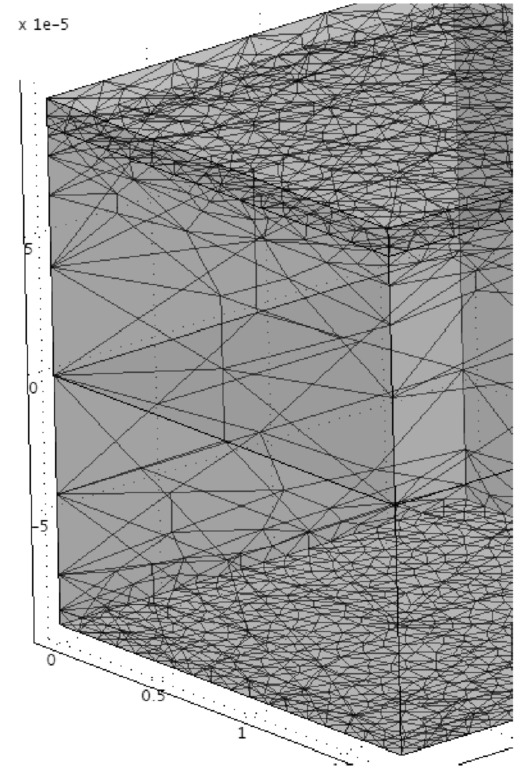
Surface resistance model - Comsol

- **Implementing in Comsol – meshing**

Regular mapped mesh - faster

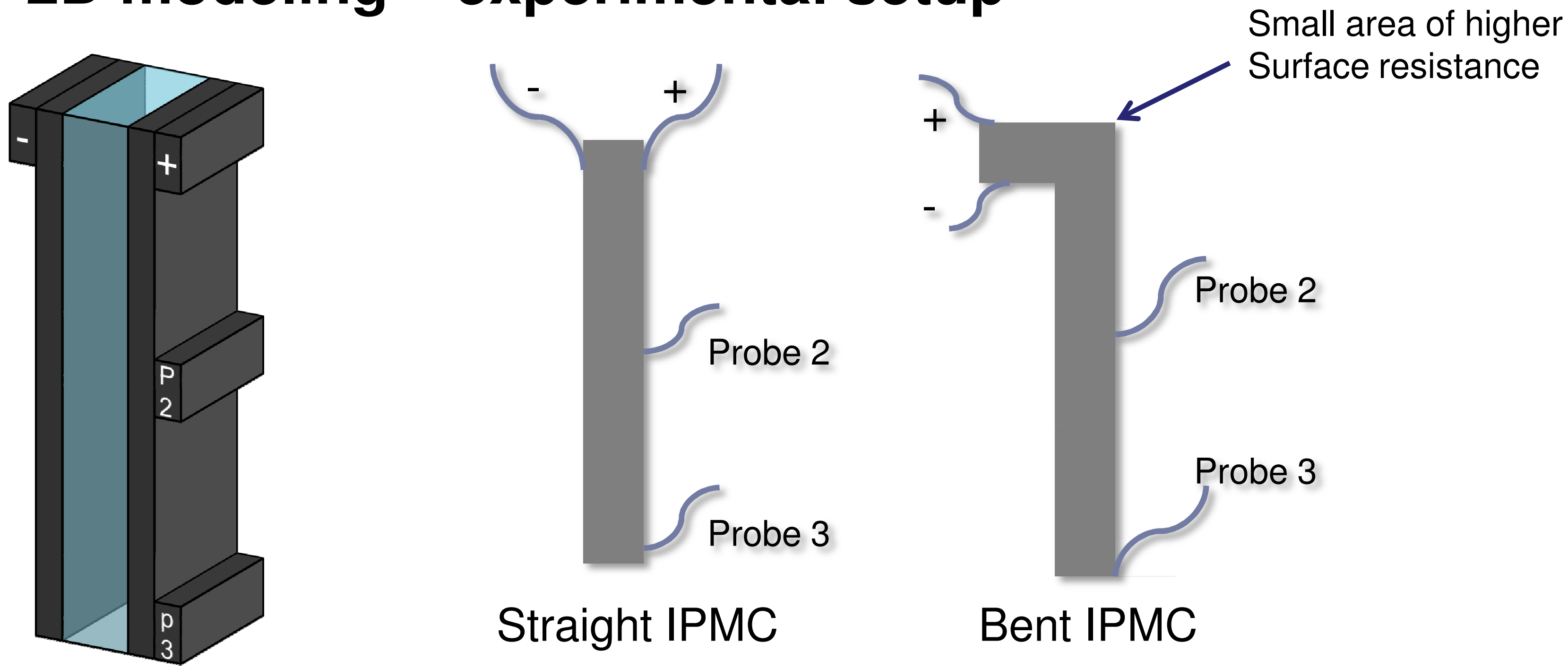


Free mesh – due to projection coupling (both for 2D and 3D simulations)

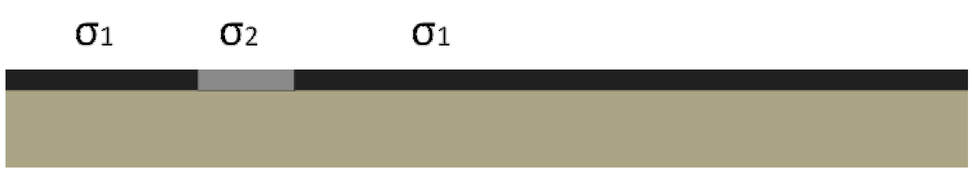


Results

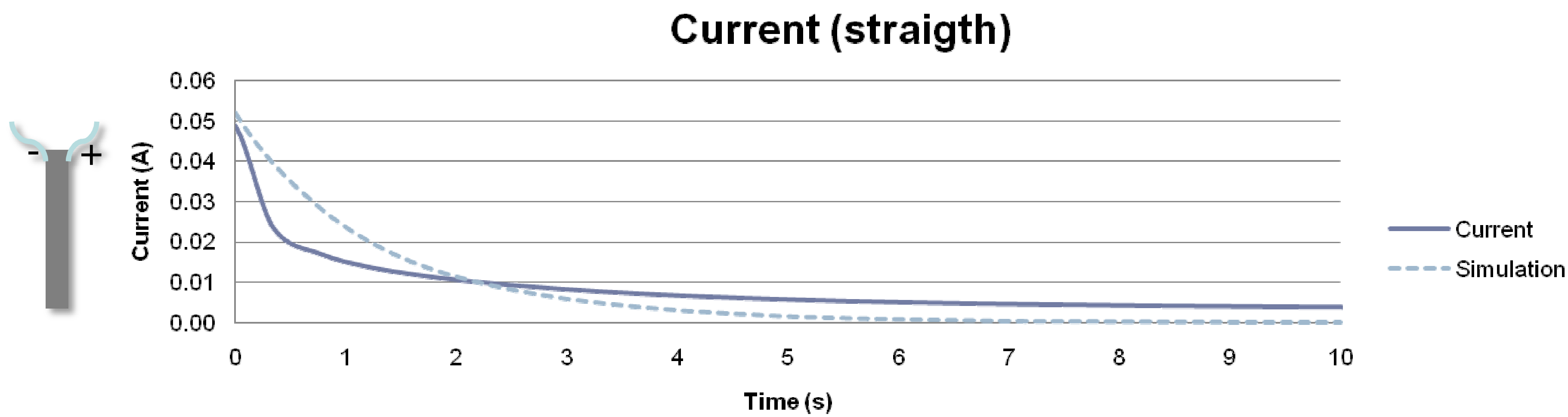
- **2D modeling – experimental setup**

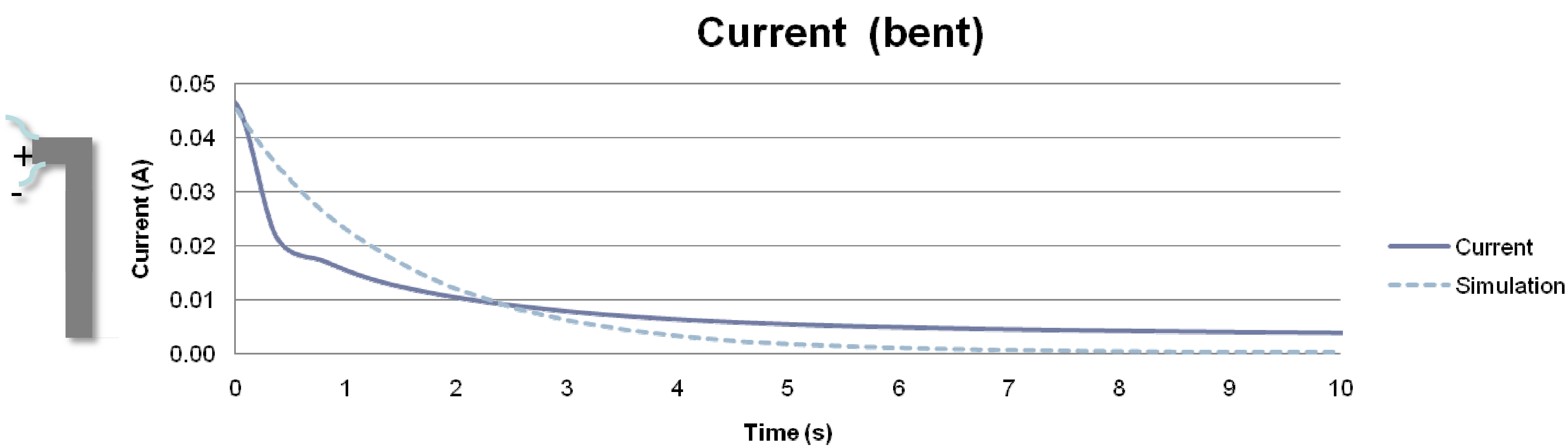


- **2D modeling – the model**



Results – 2D model, current





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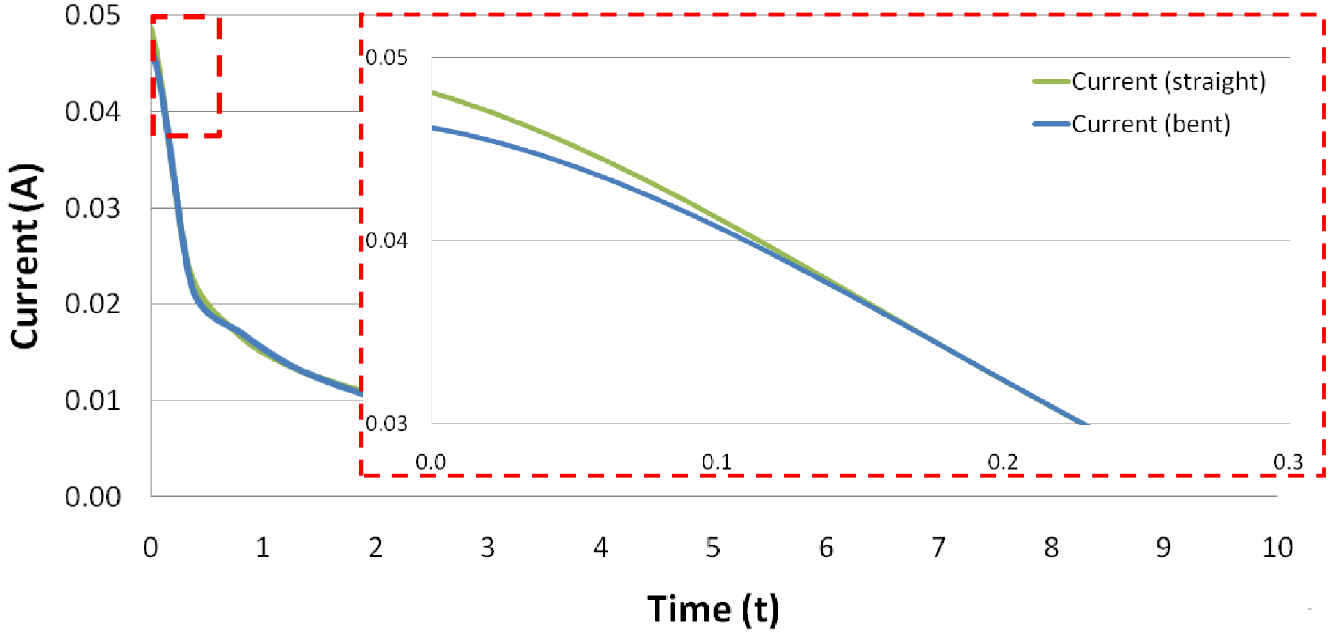
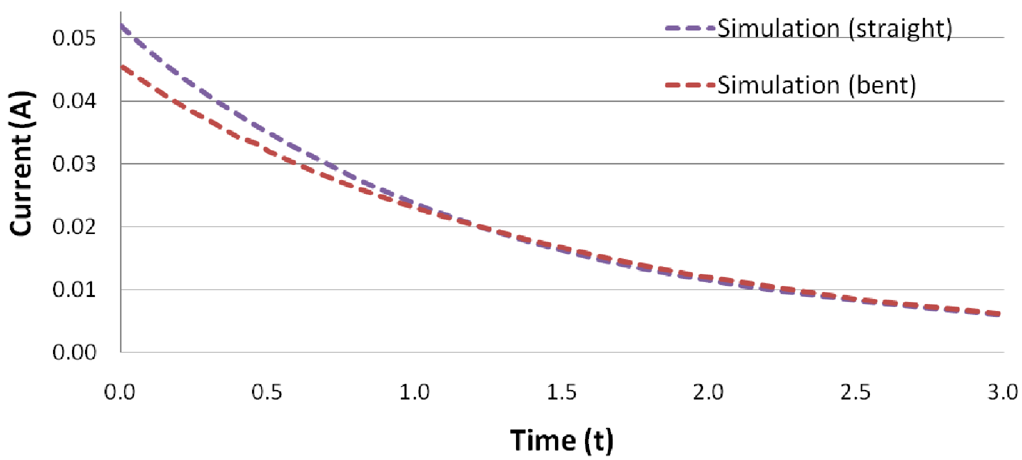
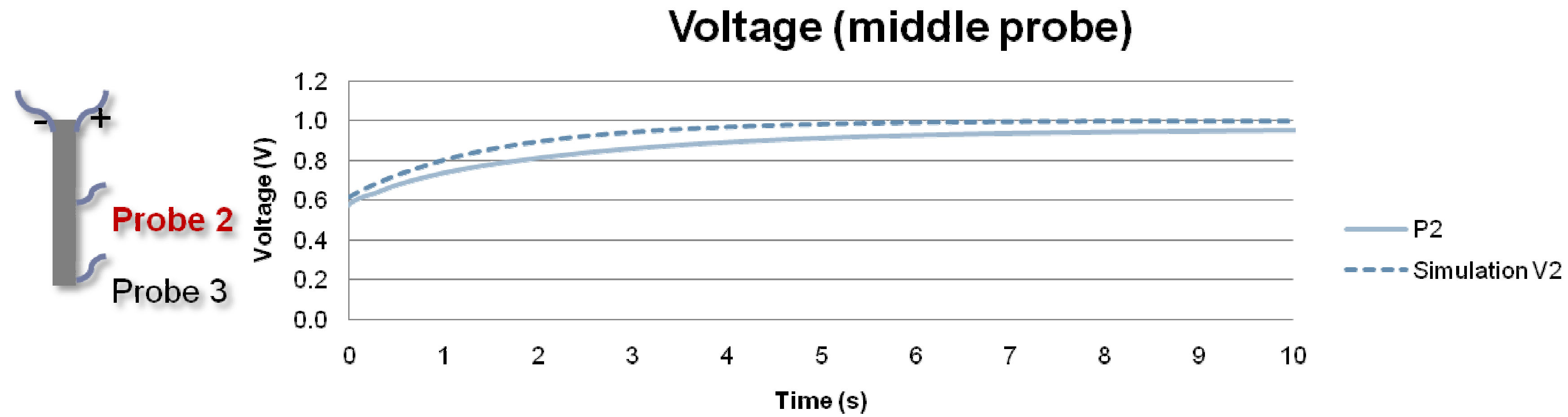
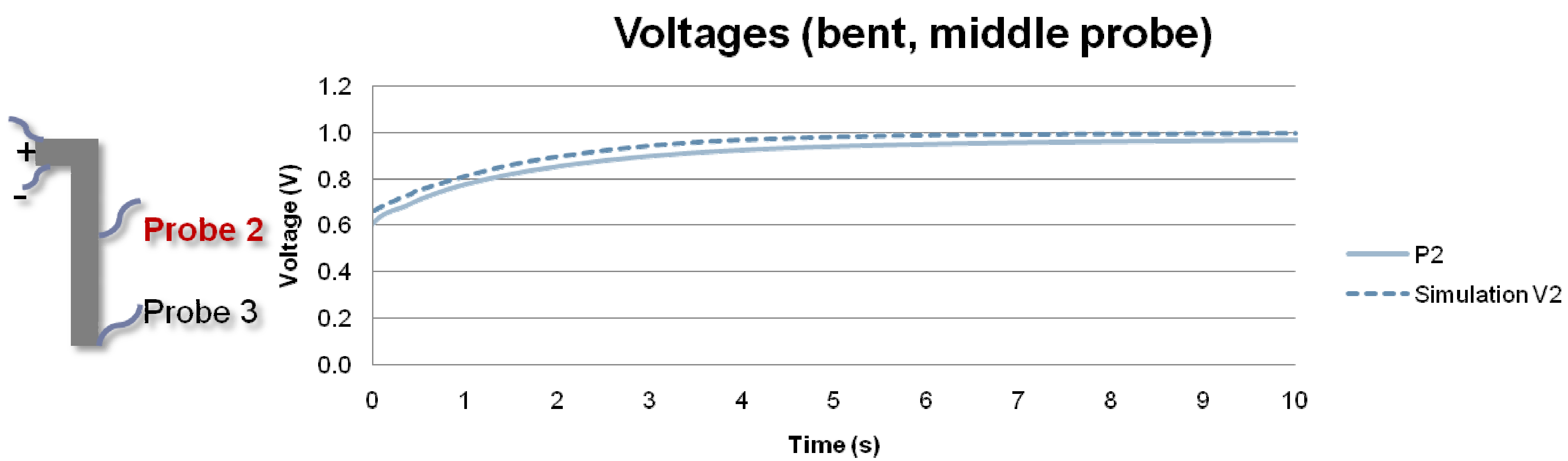
Results – 2D model, current



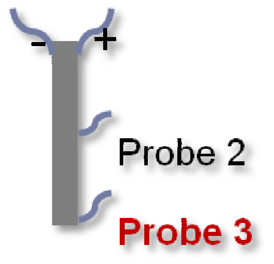


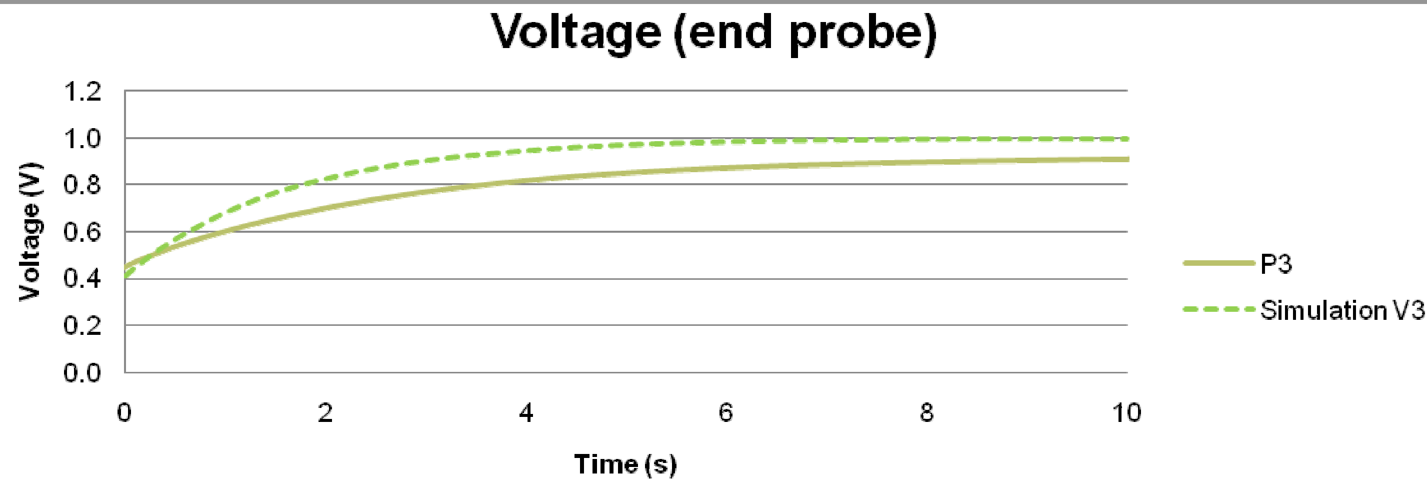
Results – 2D model, Voltage

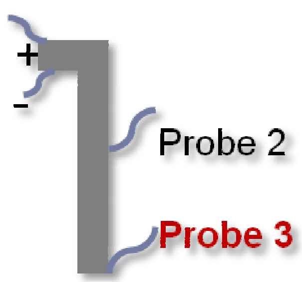


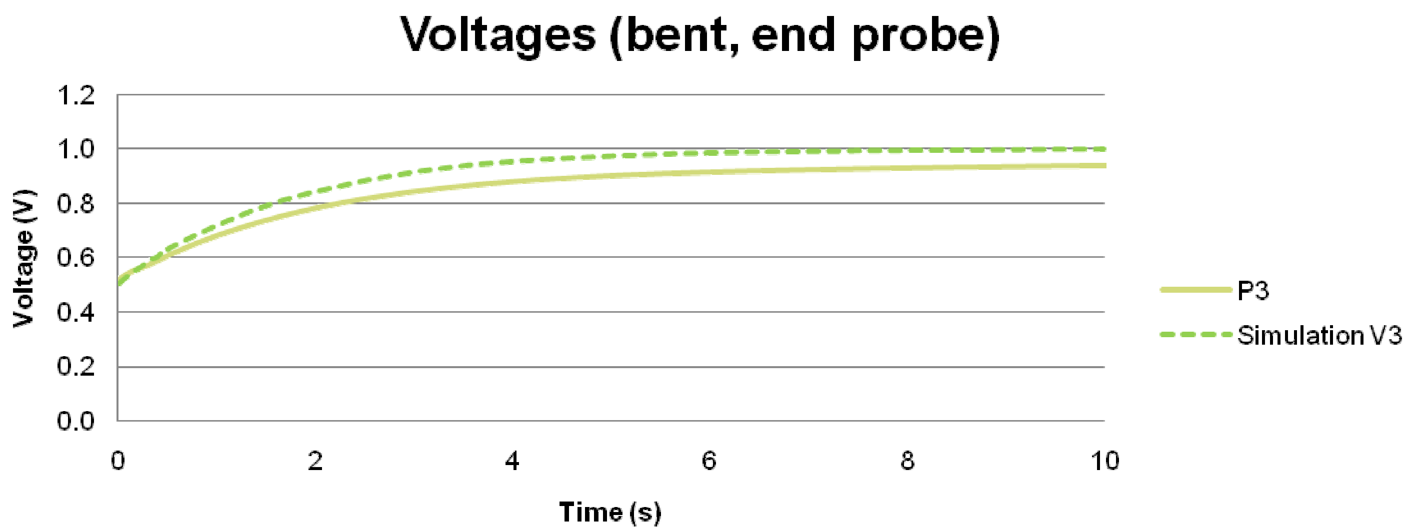


Results – 2D model, Voltage



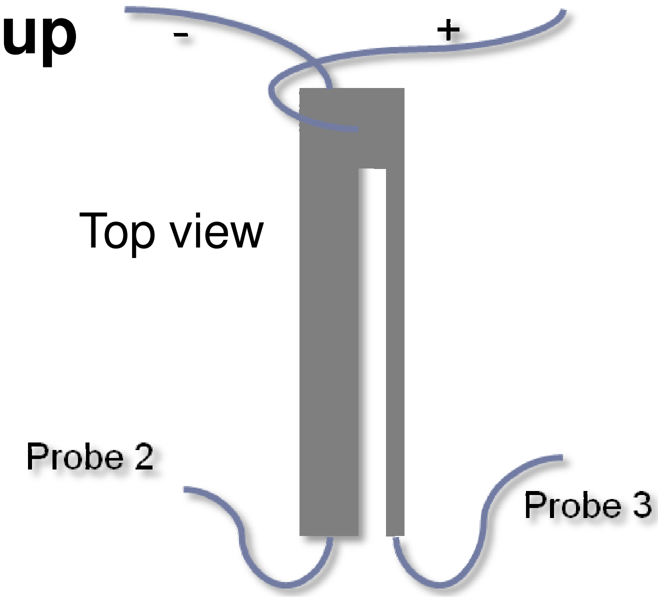




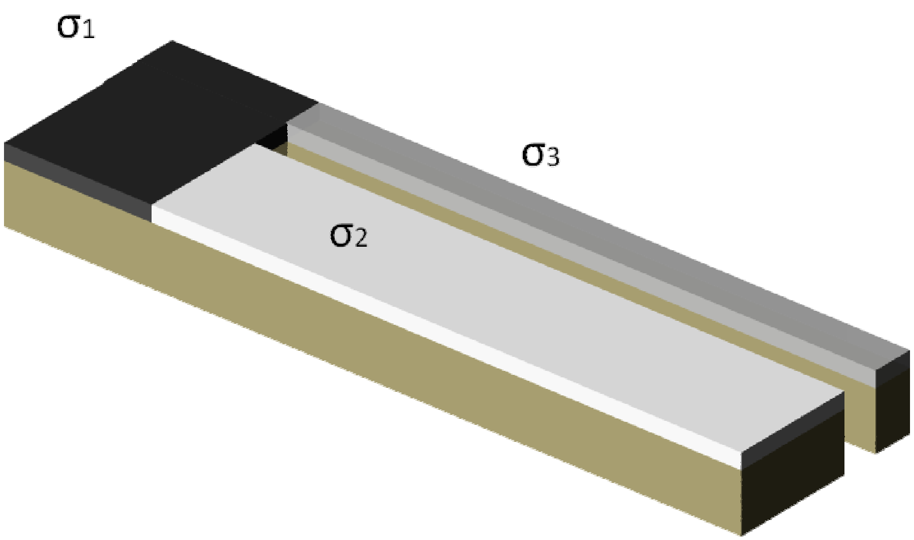


Results

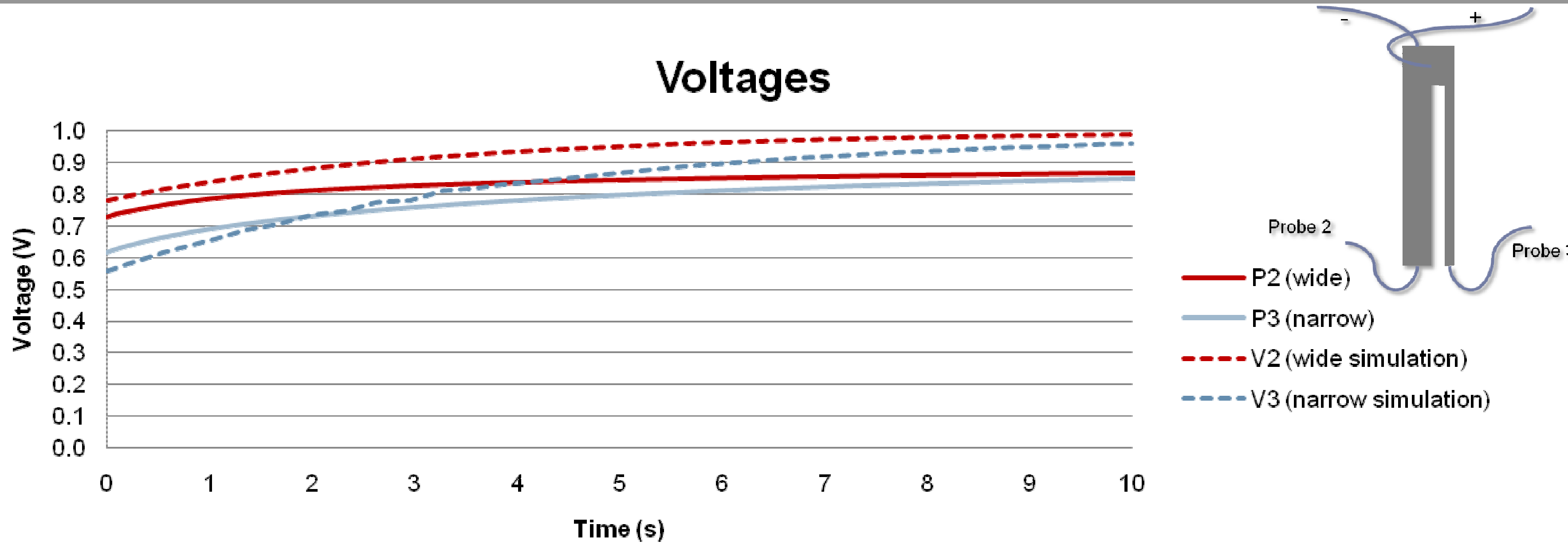
- **3D modeling – experimental setup**

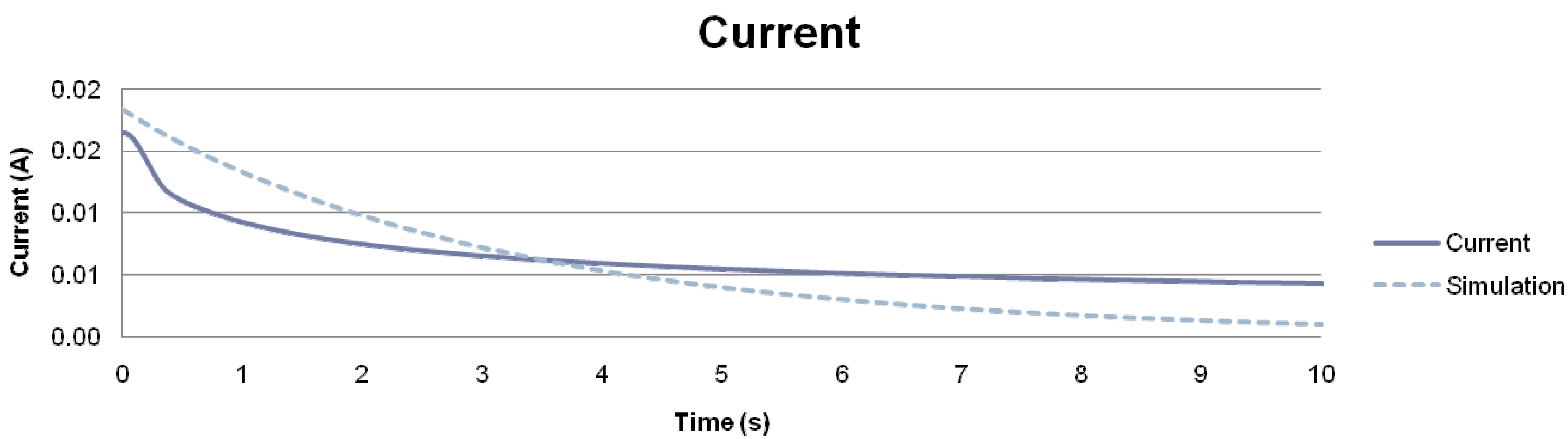


- **3D modeling – the model**
  - **Scaled model is used!**



Results – 3D model



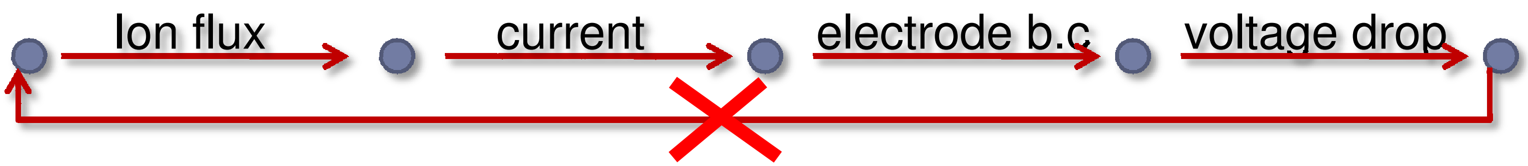


Discussion

- The results show that the model predictions are correct
  - Both electric current and the voltage drop calculations are rather realistic
  - 3D model works as well!
- Some downsides of the model
  - Time consuming calculation
  - The convergence problems due to the feedback nature of the model
- Possible solutions
  - Different solver?
  - Use time stepping instead of full time dependent solution
  - Simplify the model…

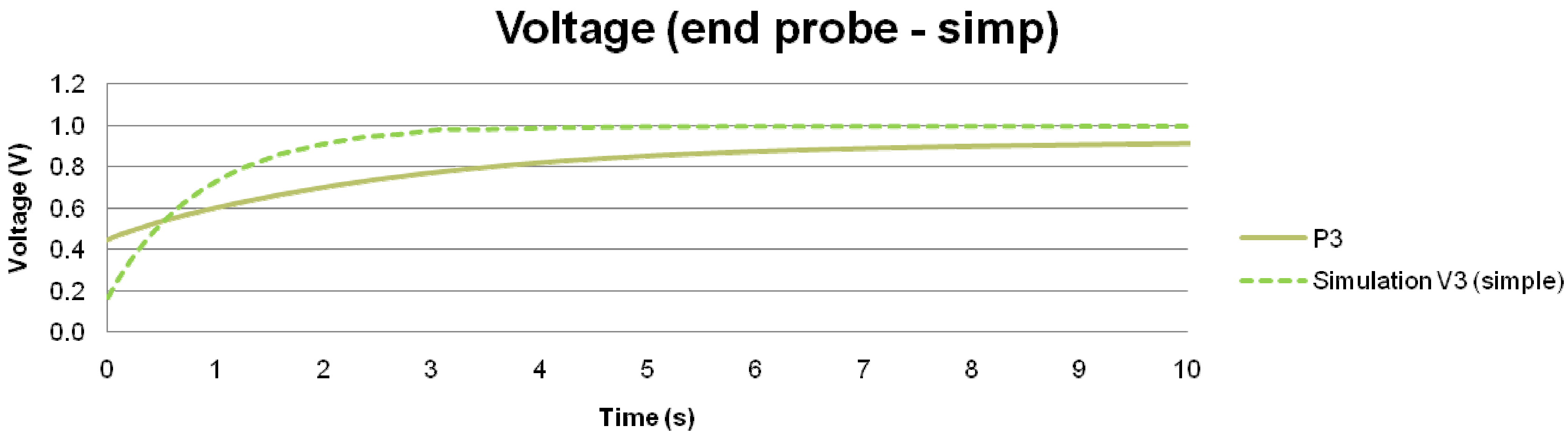
Results – simplifications

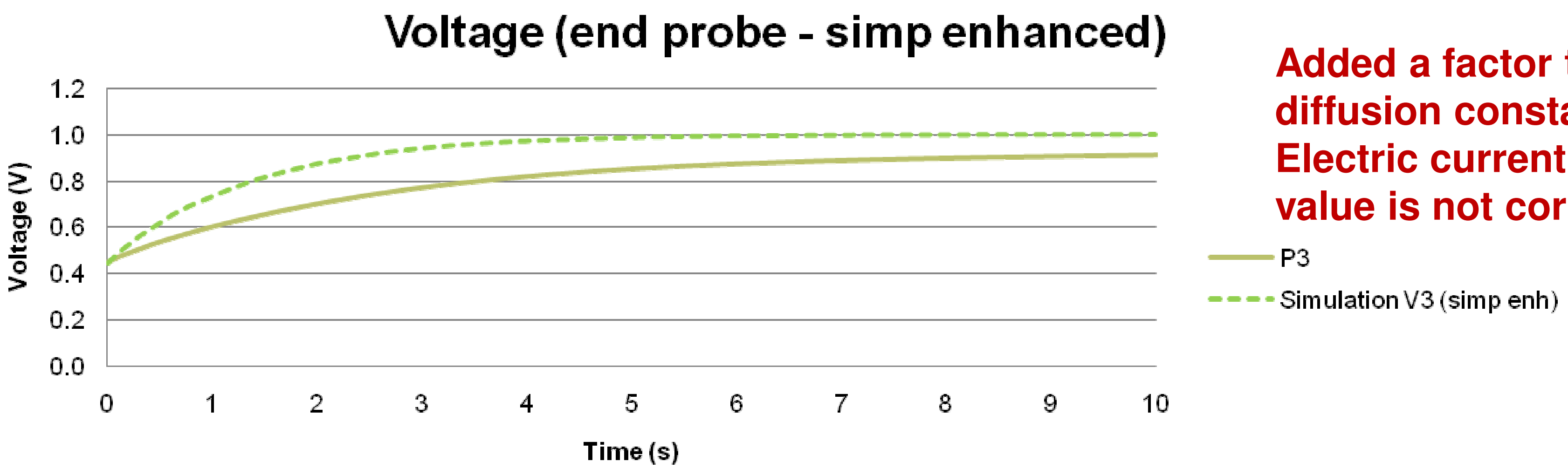
- **Loose the feedback**



  - **Better convergence**
  - **Reduced calculation time**
  - **Ionic current does cause the voltage drop on the electrodes**
  - **The voltage drop does not change the ionic current**
  - **Could be used for characterizing the surface – does not change the ionic behavior**

Results – simplified model





Added a factor to diffusion constant. Electric current value is not correct

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Conclusions

- The surface resistance model works fairly well
- The 3D scaled model was developed
  - With simple 3D IPMC, the surface could be omitted and the full scale model can be used
- Using Ramo-Shockley theorem is beneficial, when the surface resistivity plays important role
  - Surface treated IPMCs
  - More complicated structures
- Future
  - Simplify the model, reduce solution time

Acknowledgments

- **We would like to acknowledge the financial support from the following organizations:**
  - **U.S. National Science Foundation**
  - **European Science Foundation DoRa programme**

Thank you

- **Questions?**