Modeling IPMC material with dynamic surface characteristics
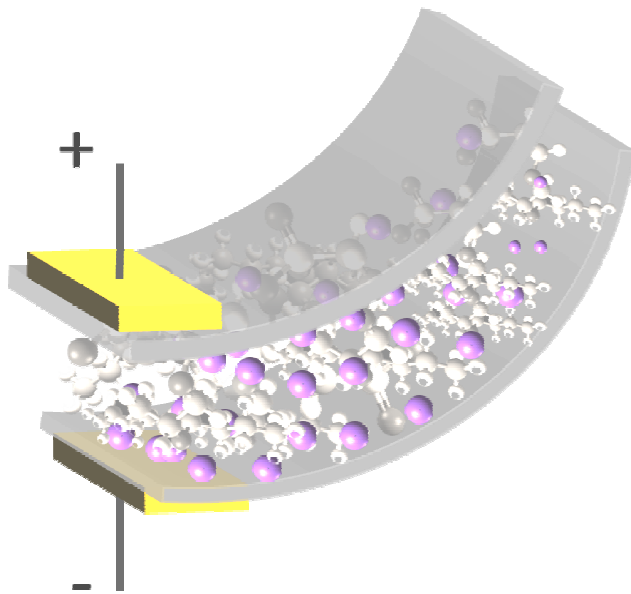
David Pugal[*#], Alvo Aabloo[#],

Kwang J. Kim[*], Youngsoo Jung[*]

[*]Active Materials and Processing Laboratory (AMPL)

Low Carbon Green Technology Laboratory (LCGTL)

Dept. of Mechanical Engineering

University of Nevada, Reno

[#]IMS Lab, Institute of Technology, Tartu University, Estonia

Outline

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

IPMC material

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

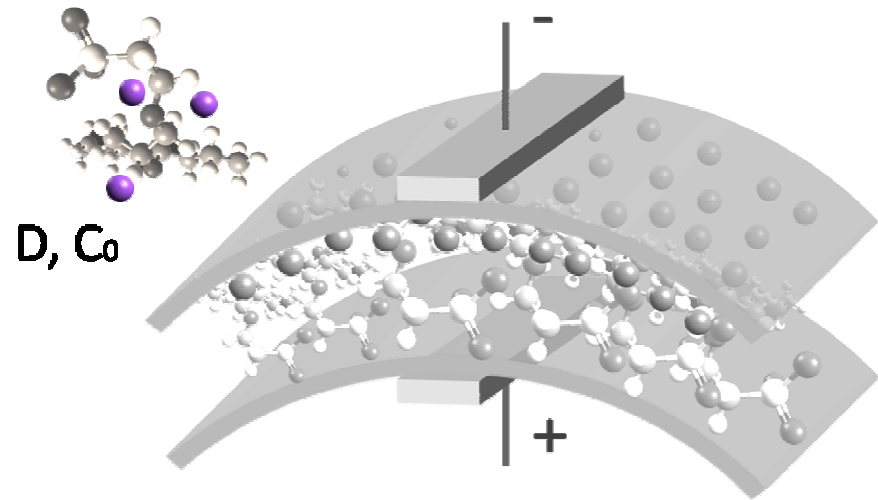Nafion™ polymer

Hydrated cation
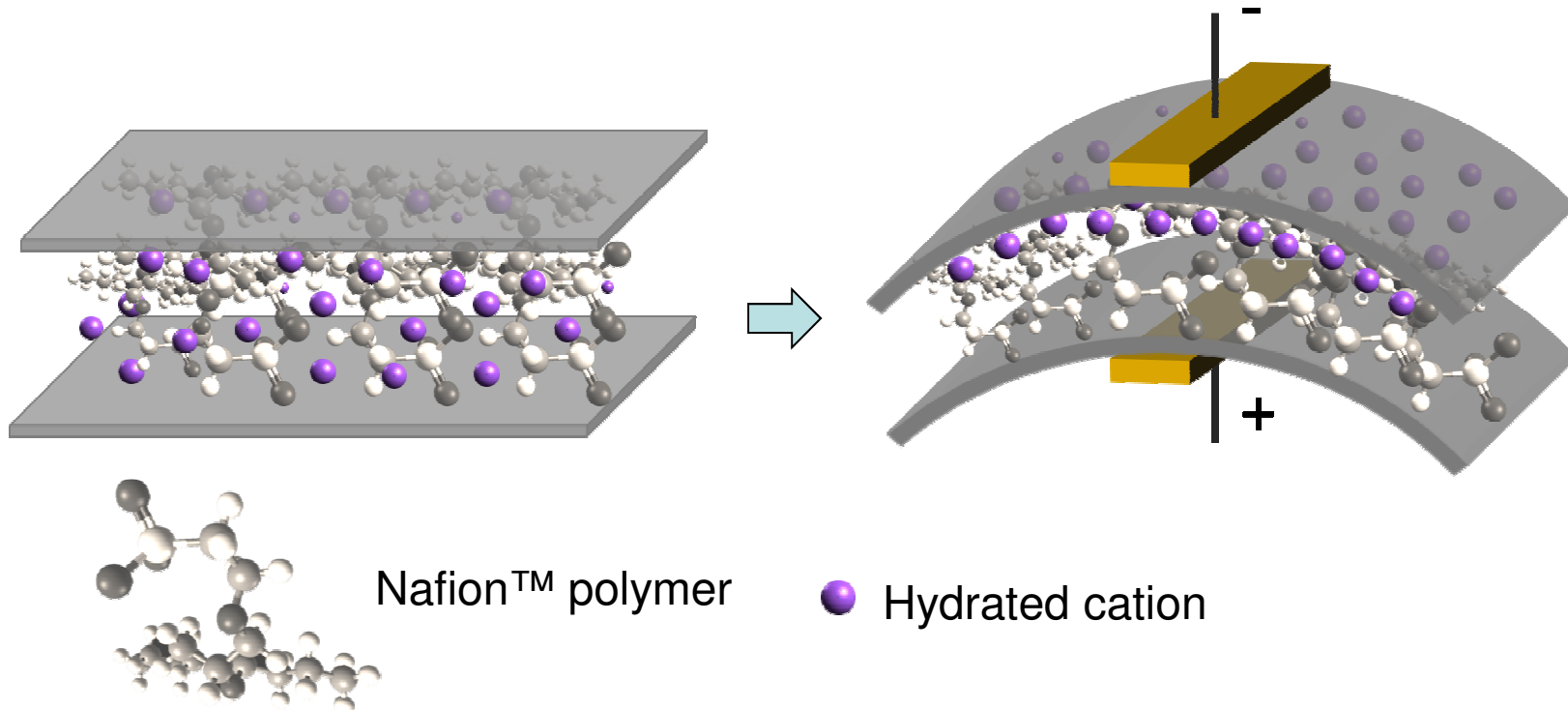
  - ### Mechanoelectrical behavior

Simple model

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

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

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

D, C$_0$

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Simple model

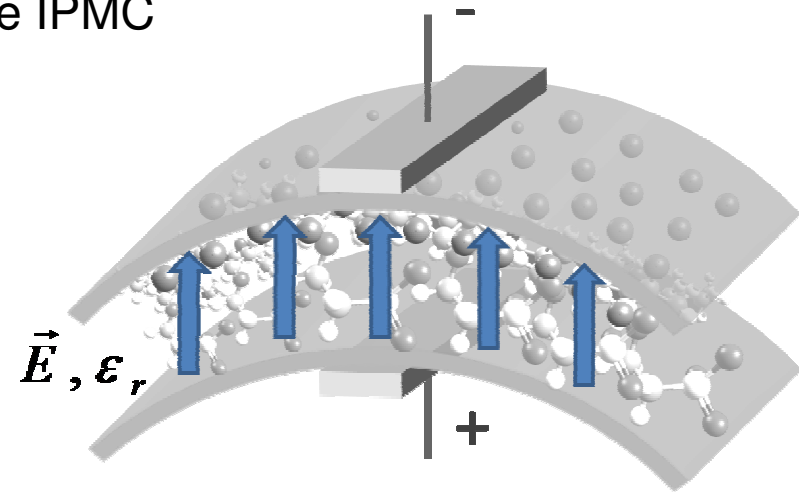- **The simple physical model:**
  - **Ion migration and diffusion** $\quad \dfrac{\partial C}{\partial t} + \nabla \cdot \left(-D\nabla C - z\mu FC\nabla\phi \right) = 0$

  - **Electric field, Poisson' equation**

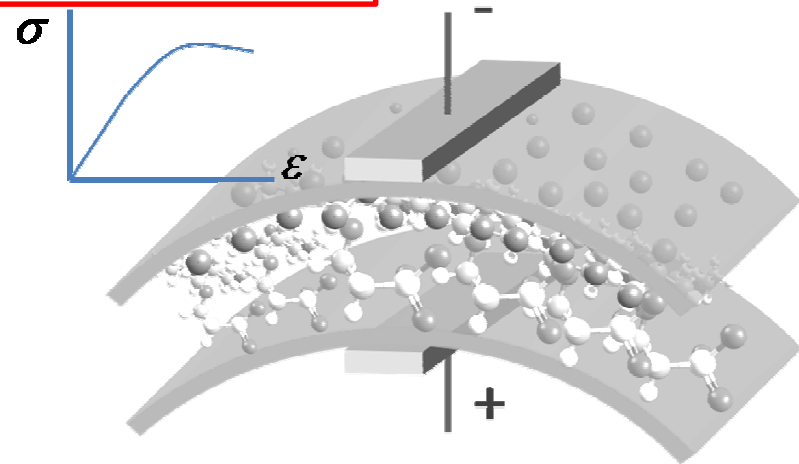$$\nabla \cdot \vec{E} = -\Delta\phi = \frac{F\rho}{\varepsilon}$$

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

$$\vec{E}, \varepsilon_r$$

Simple model

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

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

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

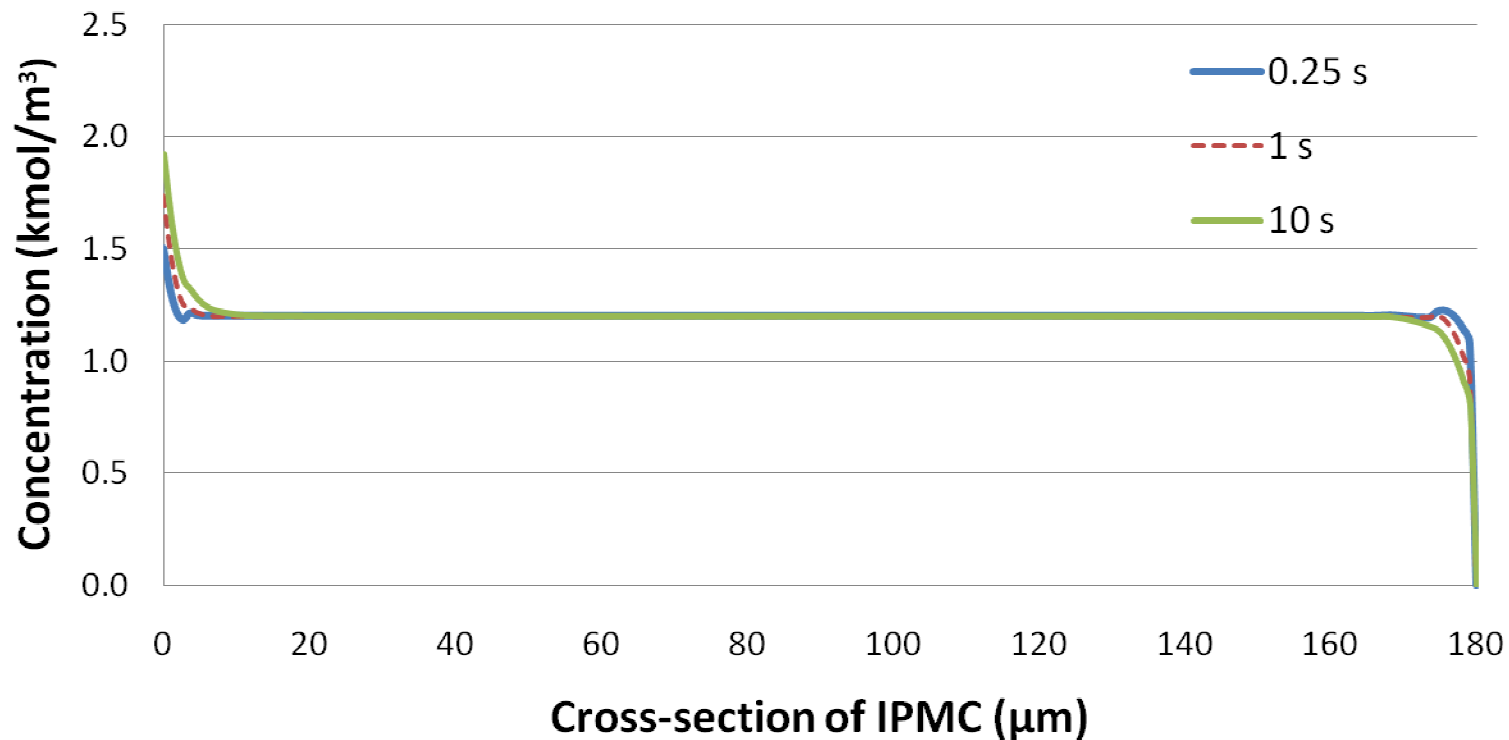$$-\nabla \cdot \sigma = \vec{F}(\rho)$$

$$\sigma = D\varepsilon$$

- Stress is related to the charge density

  - ### Not considered in this work

Concentration - Bending
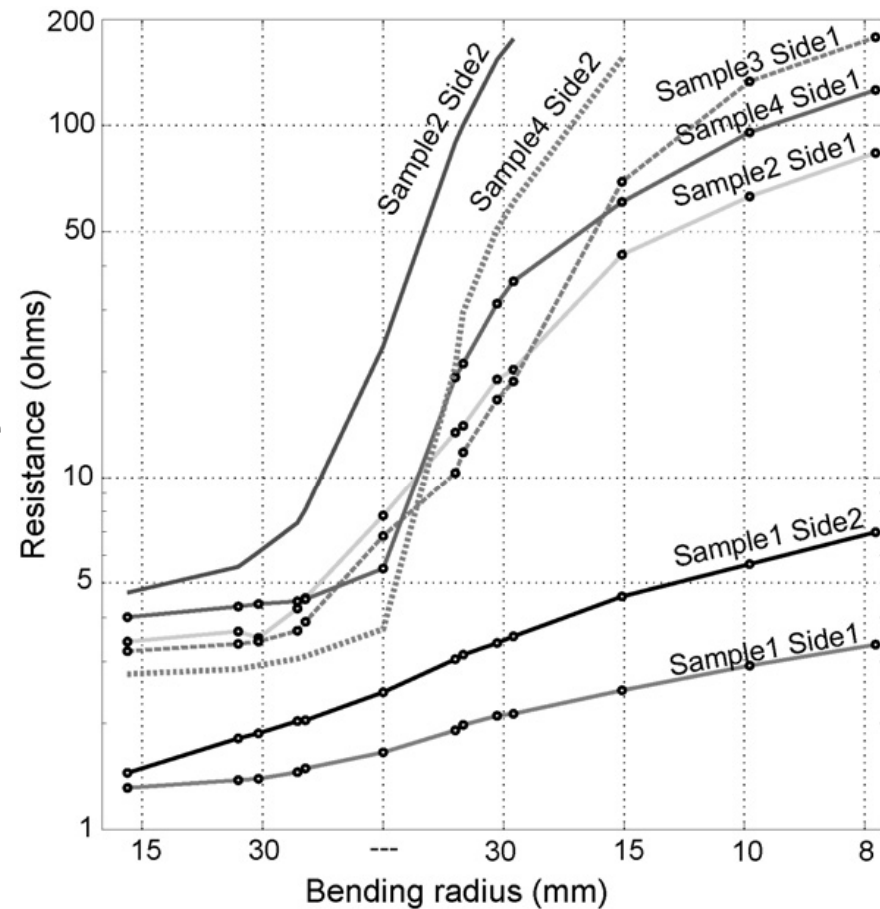
- ## Concentration graph

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

Electrode modeling - Motivation

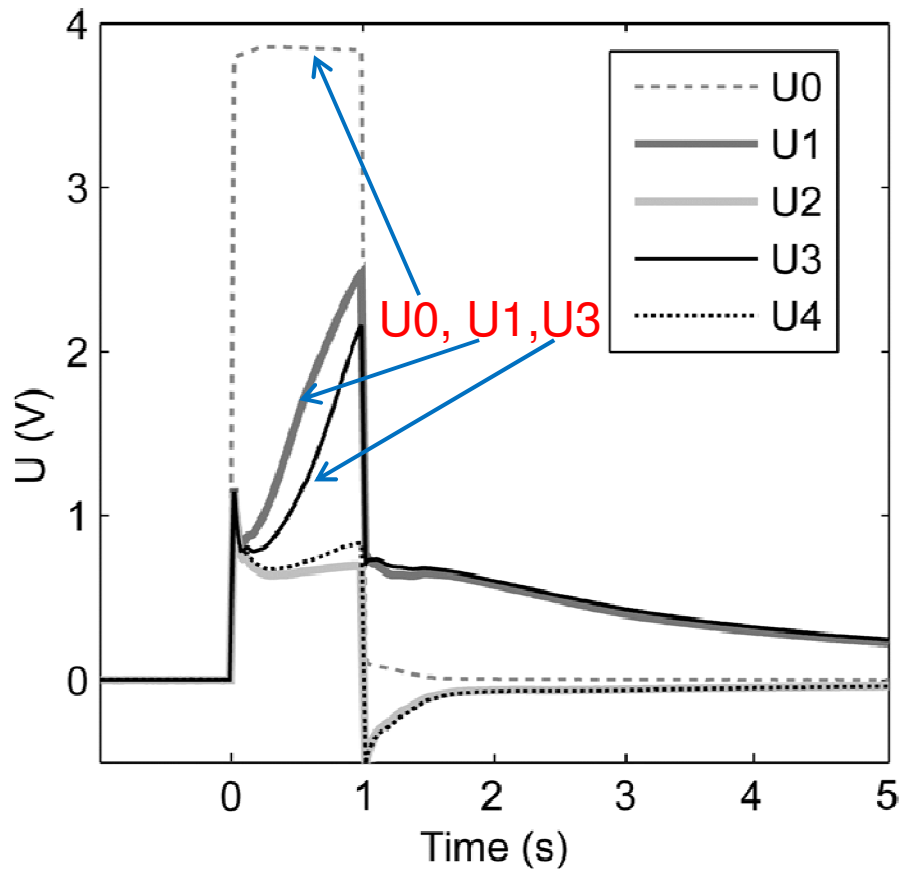- **Modeling electrode effect on the potential inside the polymer. Why?**

  1)Some samples have shown significant dynamic surface resistance

  – **Related directly to voltage drop and therefore the actuation of IPMC**

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

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Electrode modeling - Motivation

U0, U1, U3

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**

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Electrode modeling - motivation

- **Patterned electrodes**
  - **3D bending**
 - **Different areas with different surface characteristics**
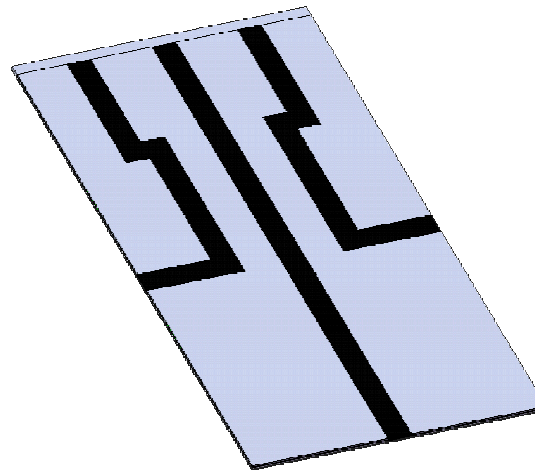
- **Electrode conductivity characterization**

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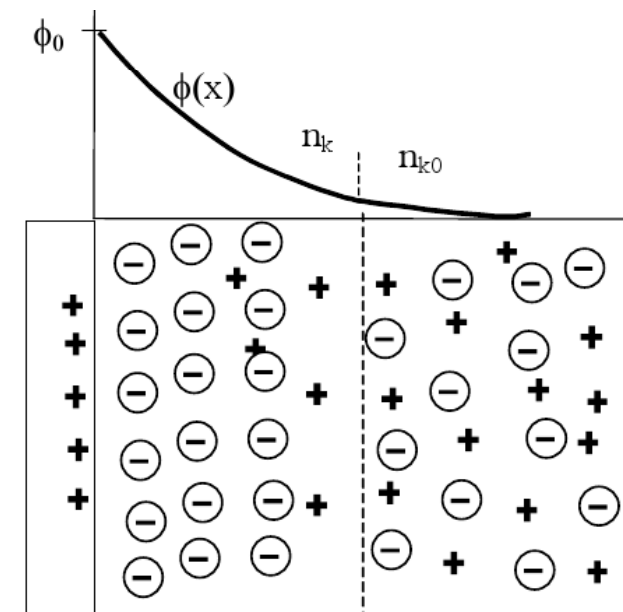
* P. Paris, M. Aints, M. Laan, and T. Plank, "Laser-induced current in air gap at atmospheric pressure," Journal of Physics D: Applied Physics 38(21), pp. 3900–3906, 2005.

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.

Courtesy of M. Laan

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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:**

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

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

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

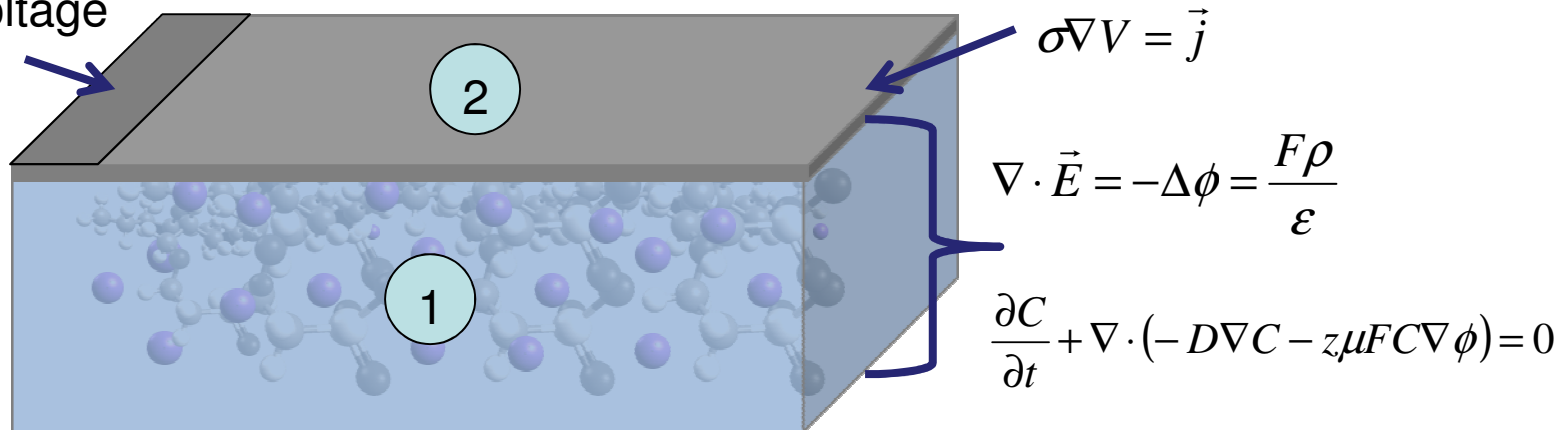⟵ Final form that is used in the simulations

Surface resistance model - Comsol

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

Input voltage

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

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

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

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

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**
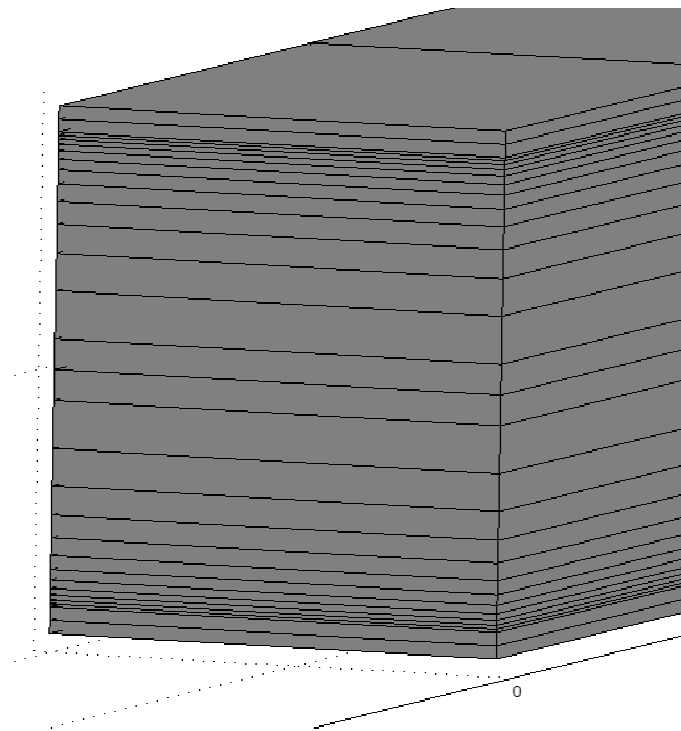
Ion flux → current → electrode b.c → voltage drop →
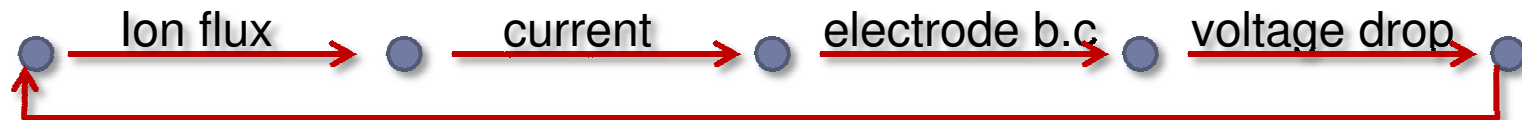
- **The voltage of the electrode model, in turn, becomes a boundary condition to the Poisson equation, which is responsible for the ion flux**
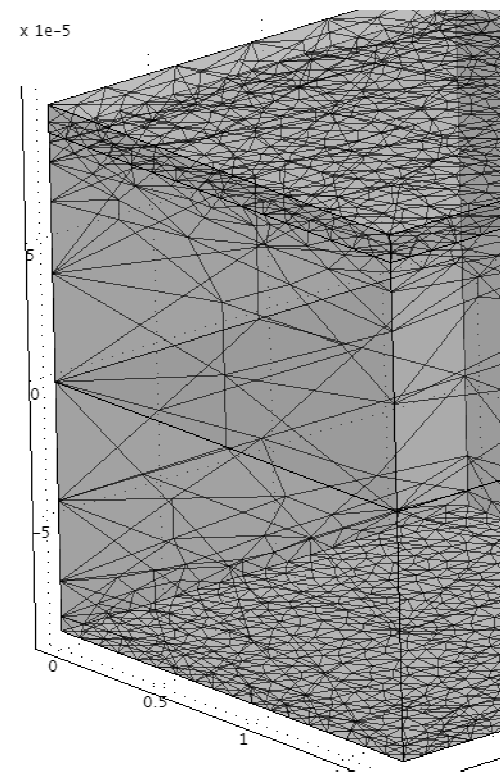
Surface resistance model - Comsol

- **Implementing in Comsol – meshing**
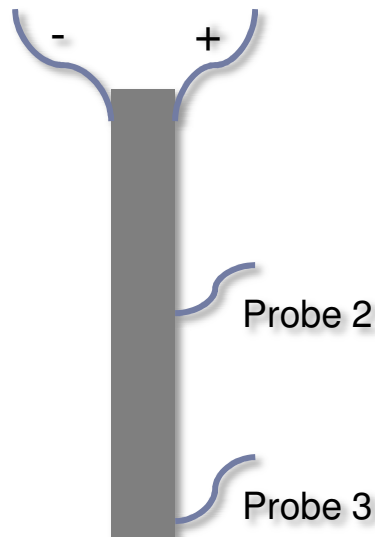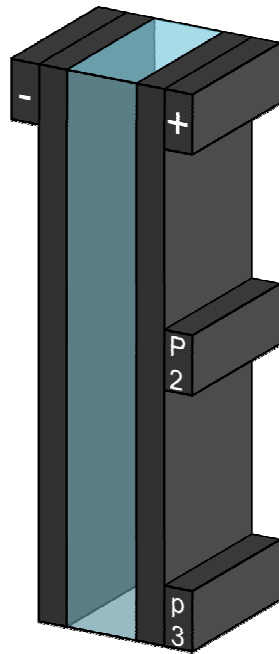
Regular mapped mesh - faster

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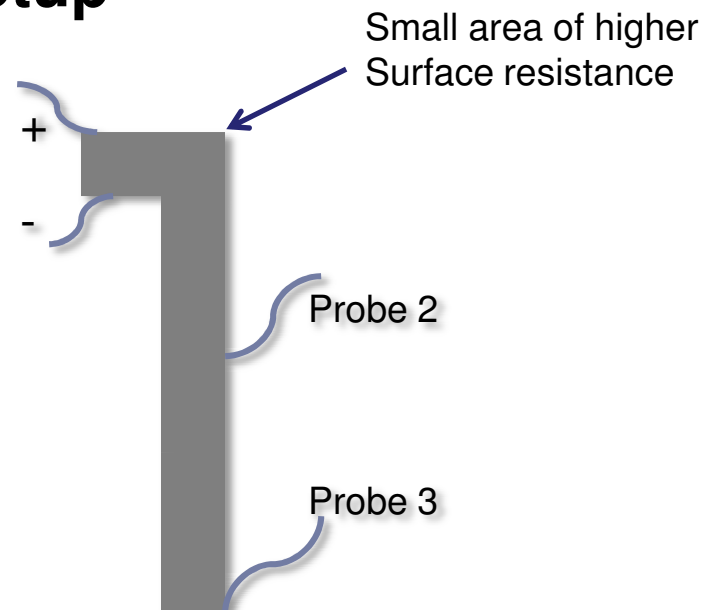(both for 2D and 3D simulations)
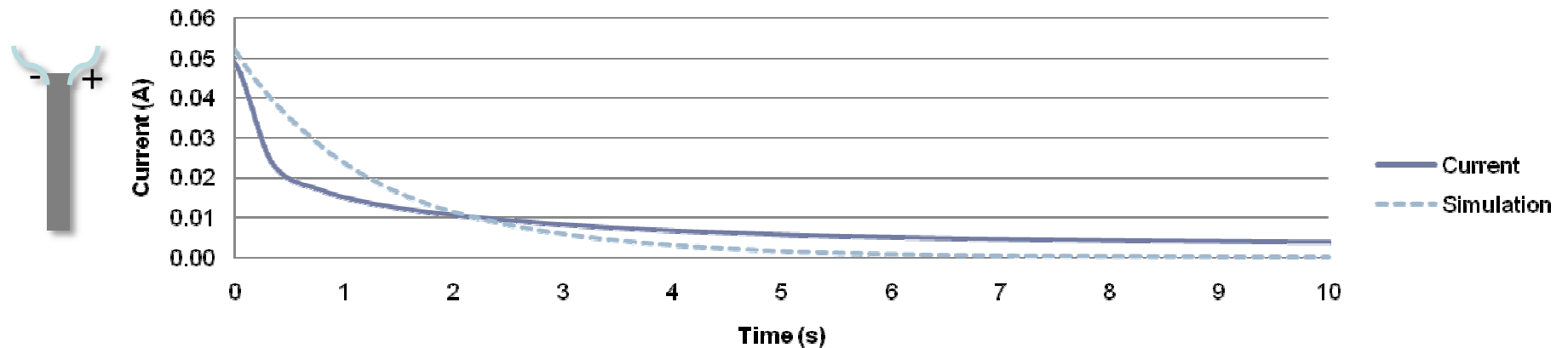
Results

- ## 2D modeling – experimental setup

Small area of higher
Surface resistance

- +

Probe 2

Probe 3

Straight IPMC

+

-

Probe 2

Probe 3

Bent IPMC

- ## 2D modeling – the model

σ_1 σ_2 σ_1

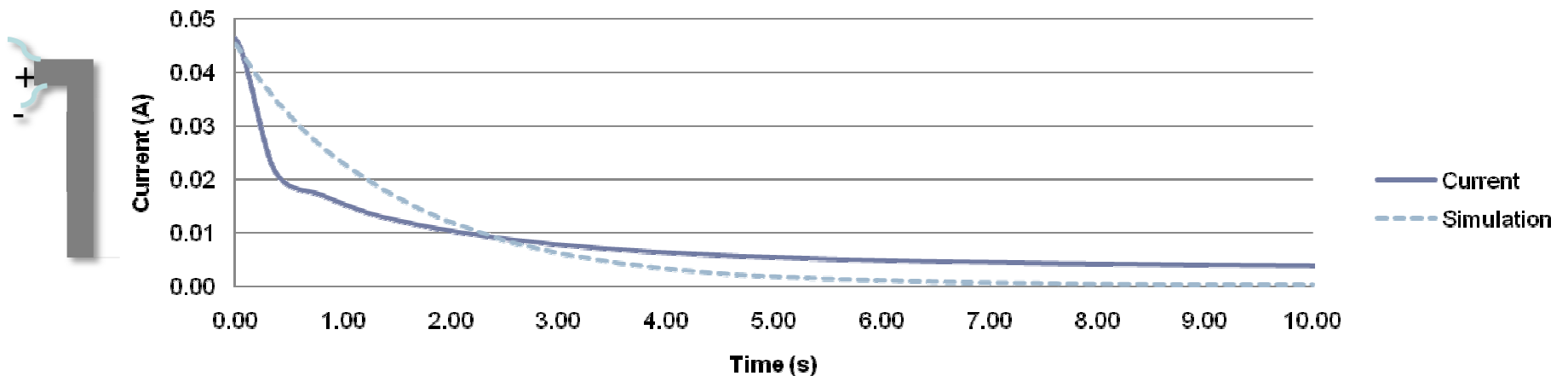*Active Materials and Processing Lab. (AMPL)*
Low Carbon Green Technology Lab. (LCGTL)

Results – 2D model, current

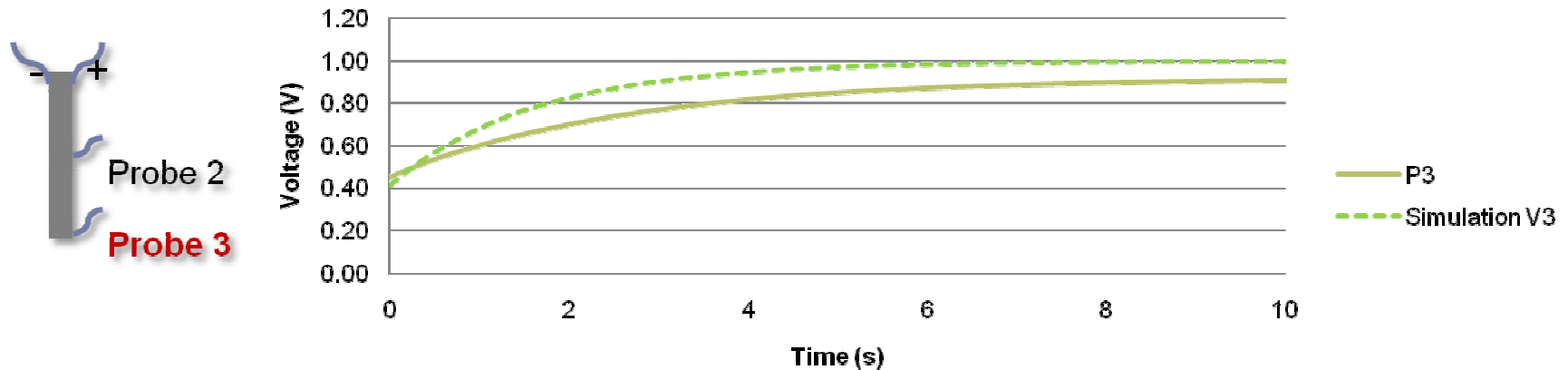

Current (straigth)

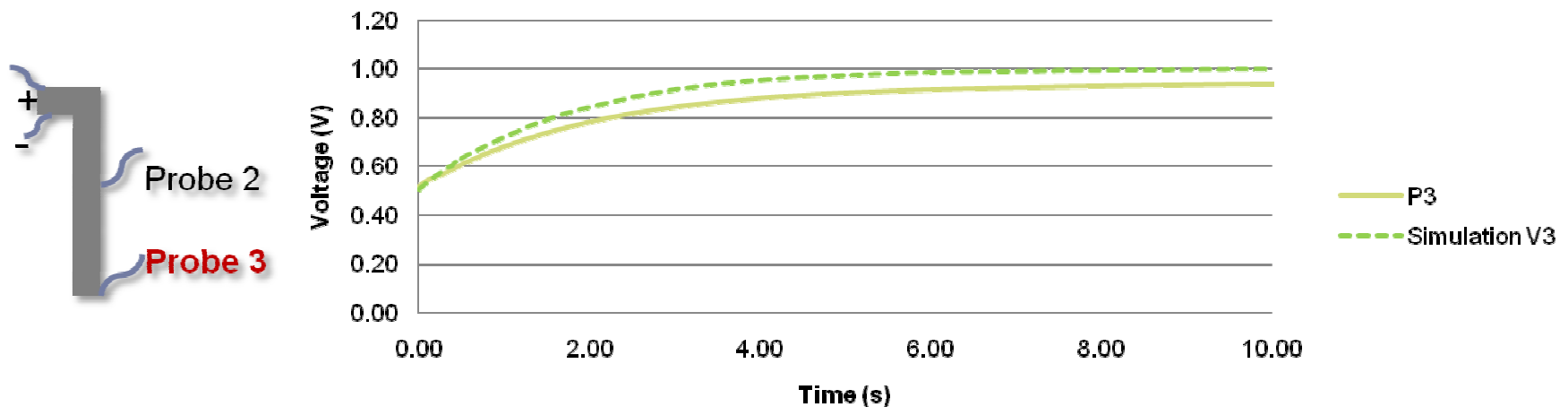Current (bent)

Results – 2D model, Voltage
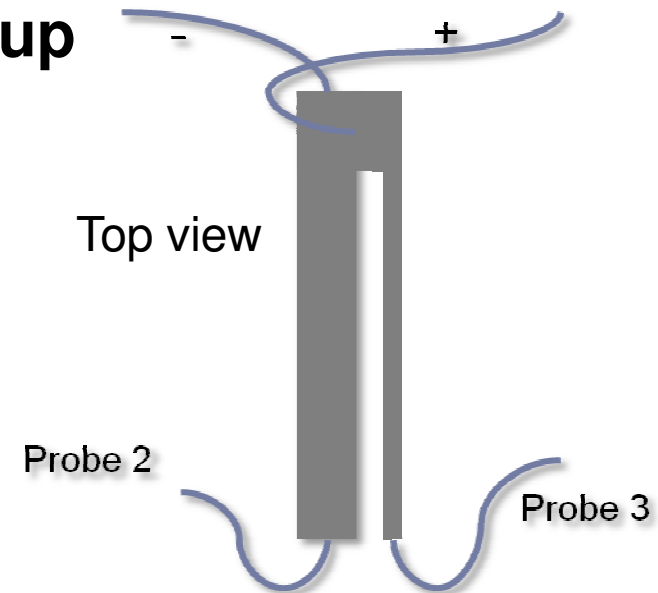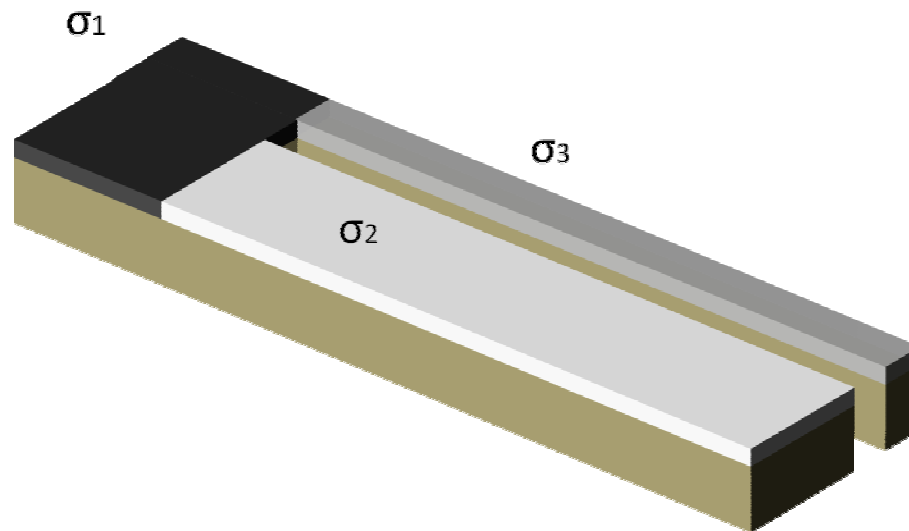
Results – 2D model, Voltage

Voltage (end probe)

Voltages (bent, end probe)

Results
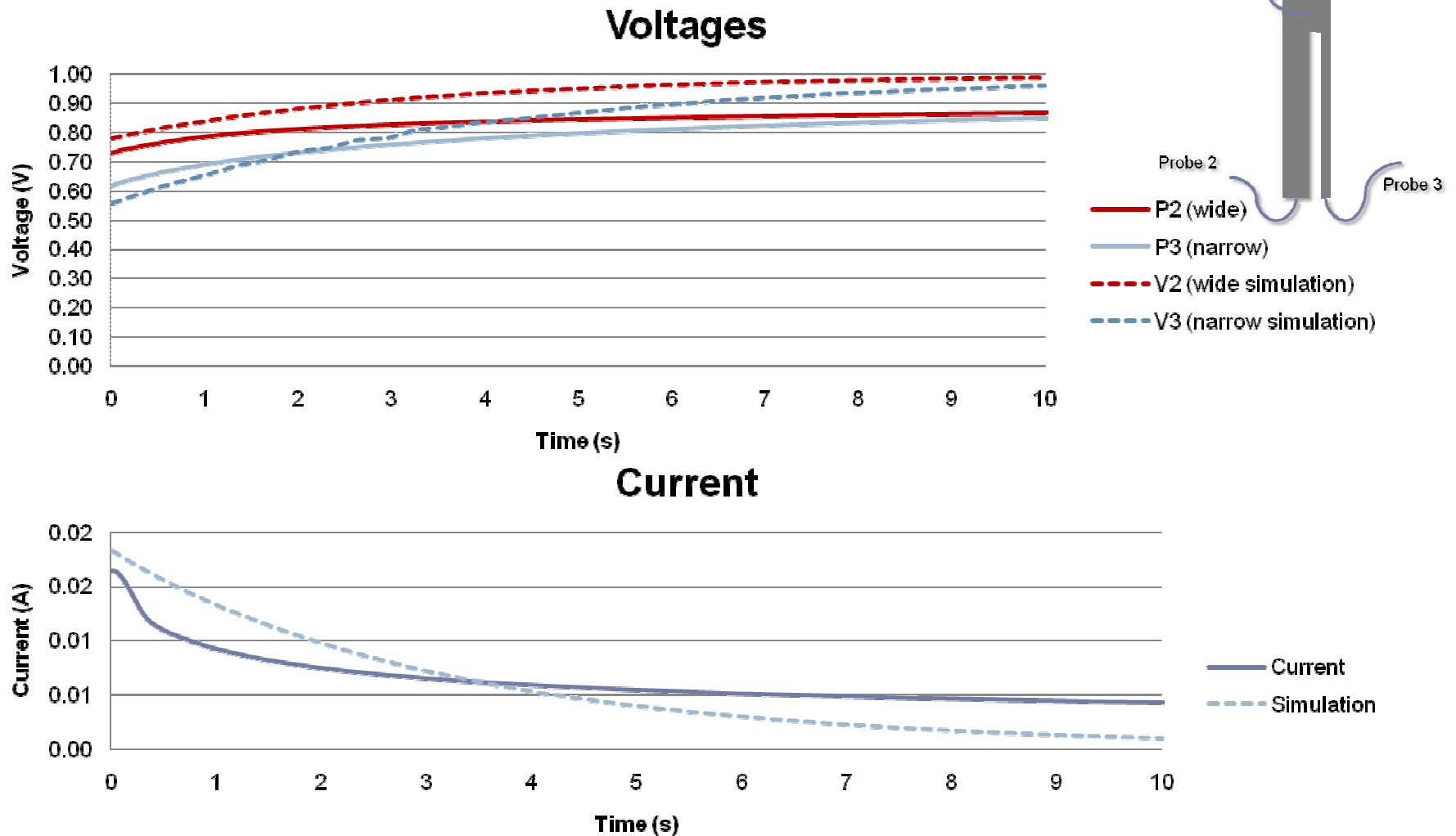
- ## 3D modeling – experimental setup

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

Top view

$-$ $+$

Probe 2

Probe 3

σ_1

σ_3

σ_2

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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…

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Results – simplifications

- **Loose the feedback**

Ion flux → current → electrode b.c → voltage drop
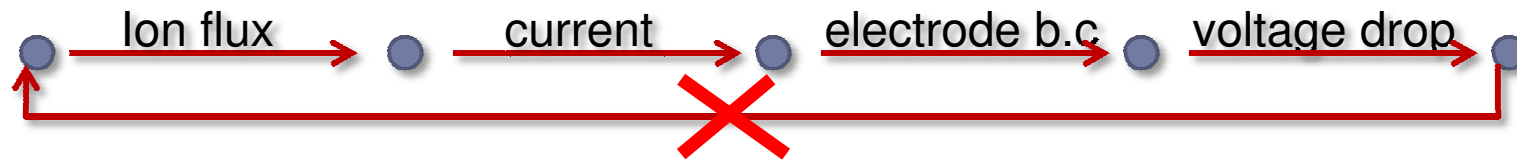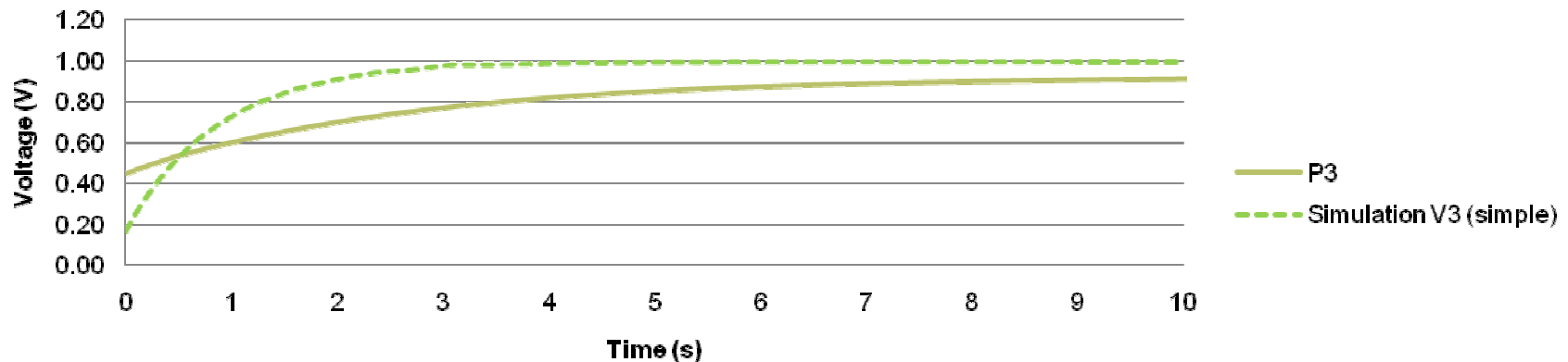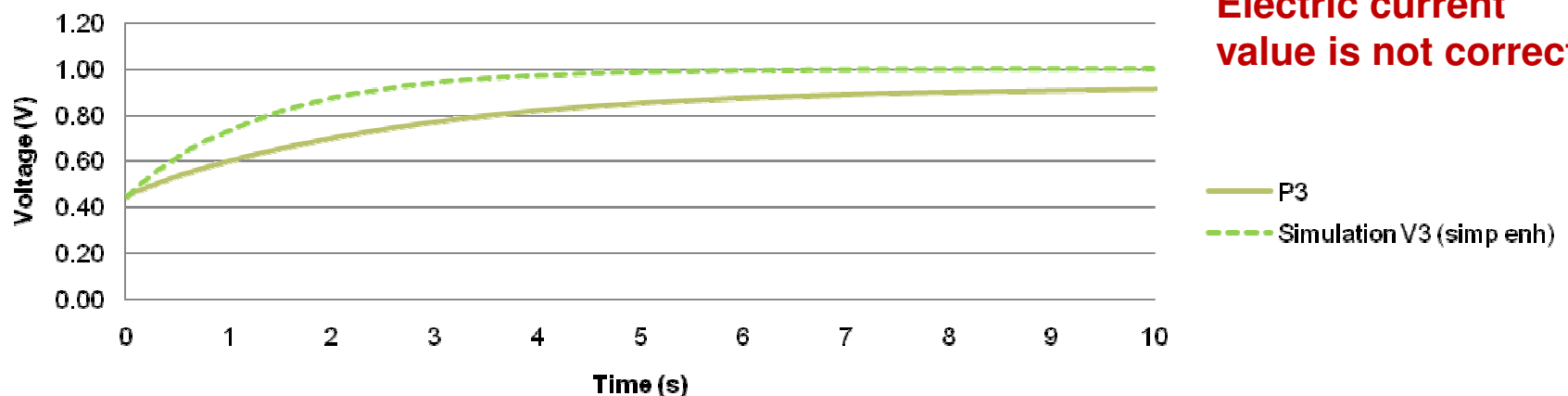
  – **Better convergence**
  – **Reduced calculation time**
  – **Ionic current does cause the voltage drop on the electrodes**
  – **The voltage drop does not change the ionic current**
  – **Could be used for characterizing the surface – does not change the ionic behavior**

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Results – simplified model

Voltage (end probe - simp)

— P3
---- Simulation V3 (simple)

Voltage (end probe - simp enhanced)

— P3
---- Simulation V3 (simp enh)

**Changed 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**

No. 5

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DoRa
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Thank you

- **Questions?**

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