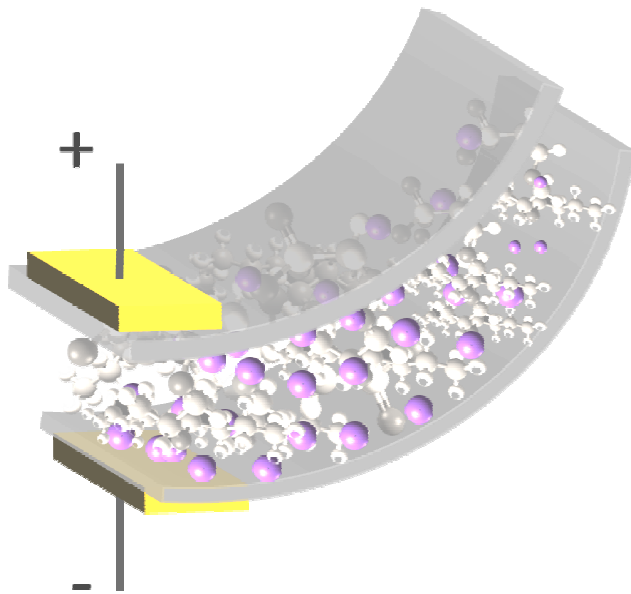


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Modeling IPMC material with dynamic surface characteristics



**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

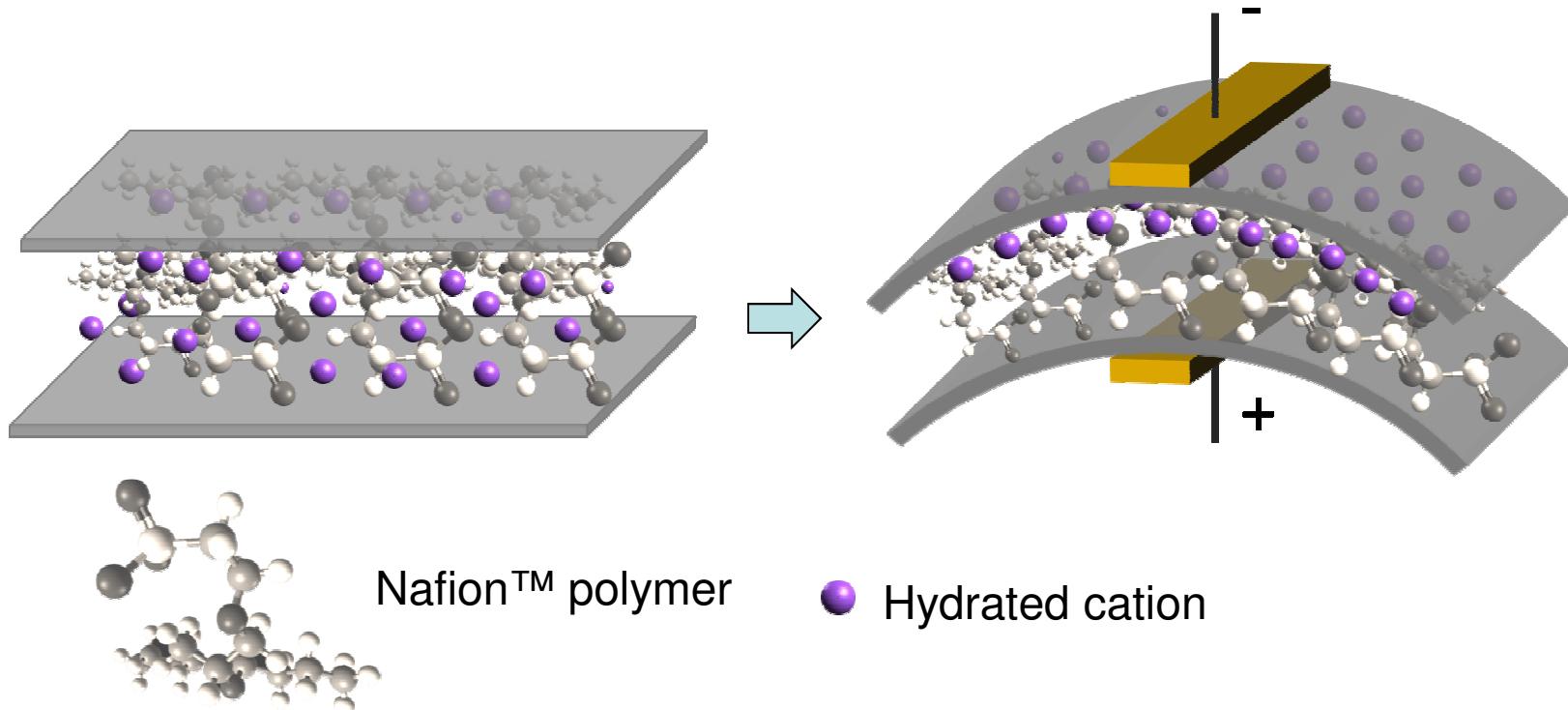
[#]IMS Lab, Institute of Technology, Tartu University, Estonia

Outline

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

IPMC material

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



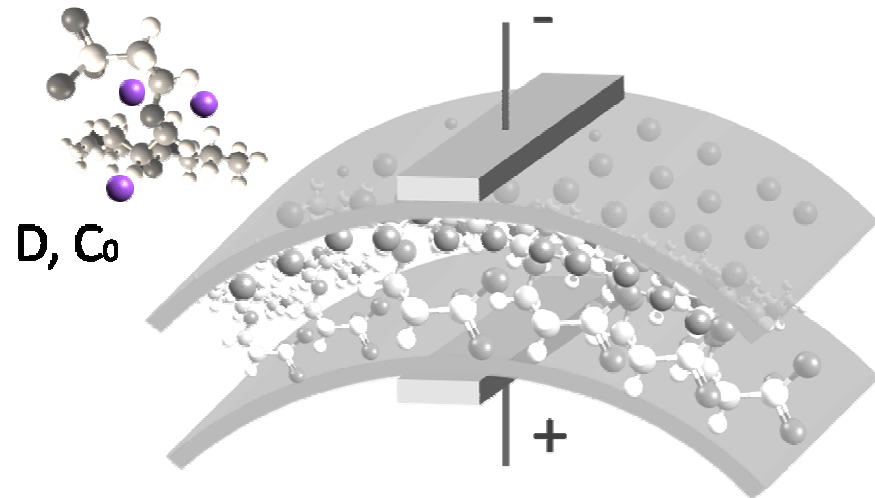
- Mechanoelectrical behavior

Simple model

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

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

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



Simple model

- **The simple physical model:**

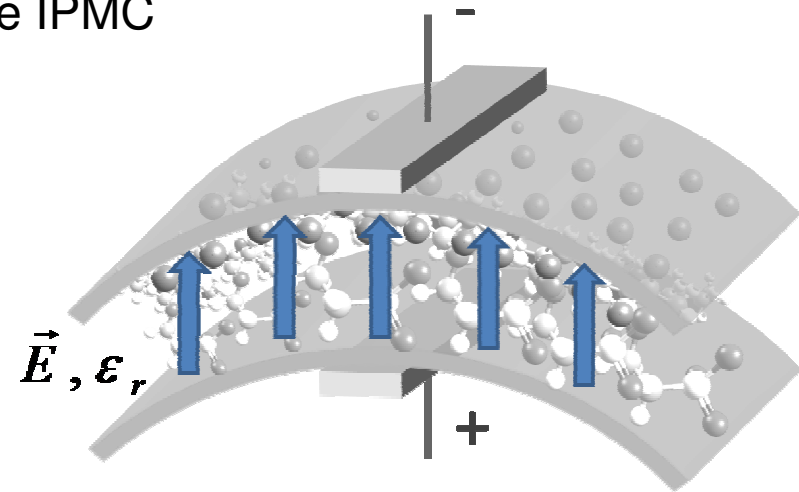
- Ion migration and diffusion

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

- **Electric field, Poisson' equation**

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

- 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

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

- Electric field, Poisson' equation

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

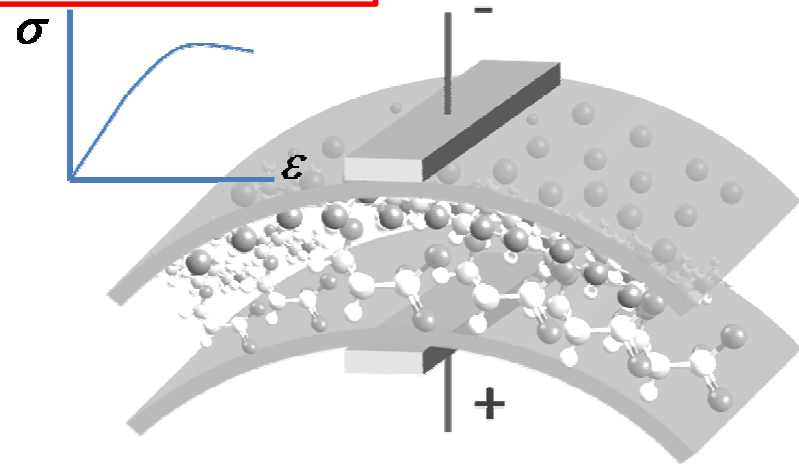
- **Stress-strain**

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

$$\sigma = D\varepsilon$$

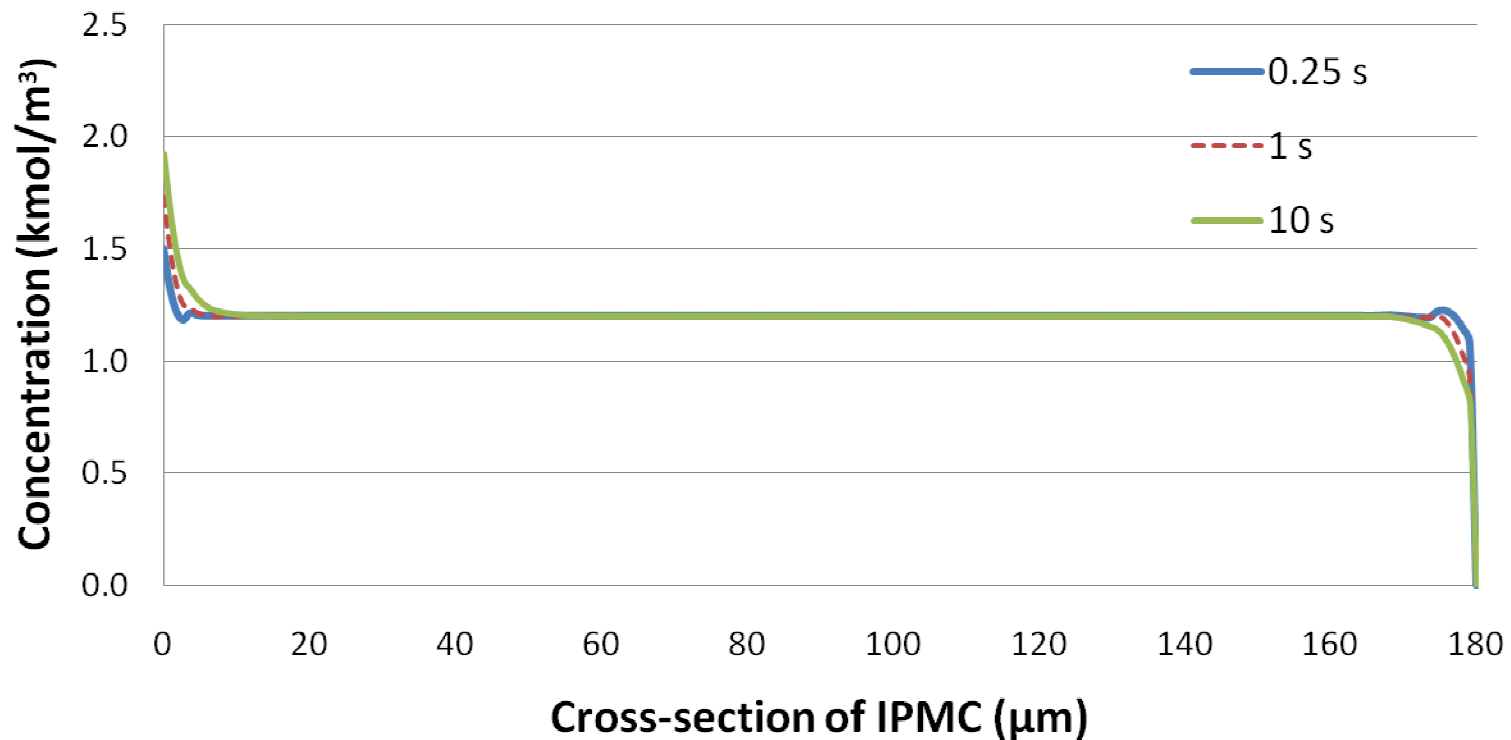
- Stress is related to the charge density

- **Not considered in this work**



Concentration - Bending

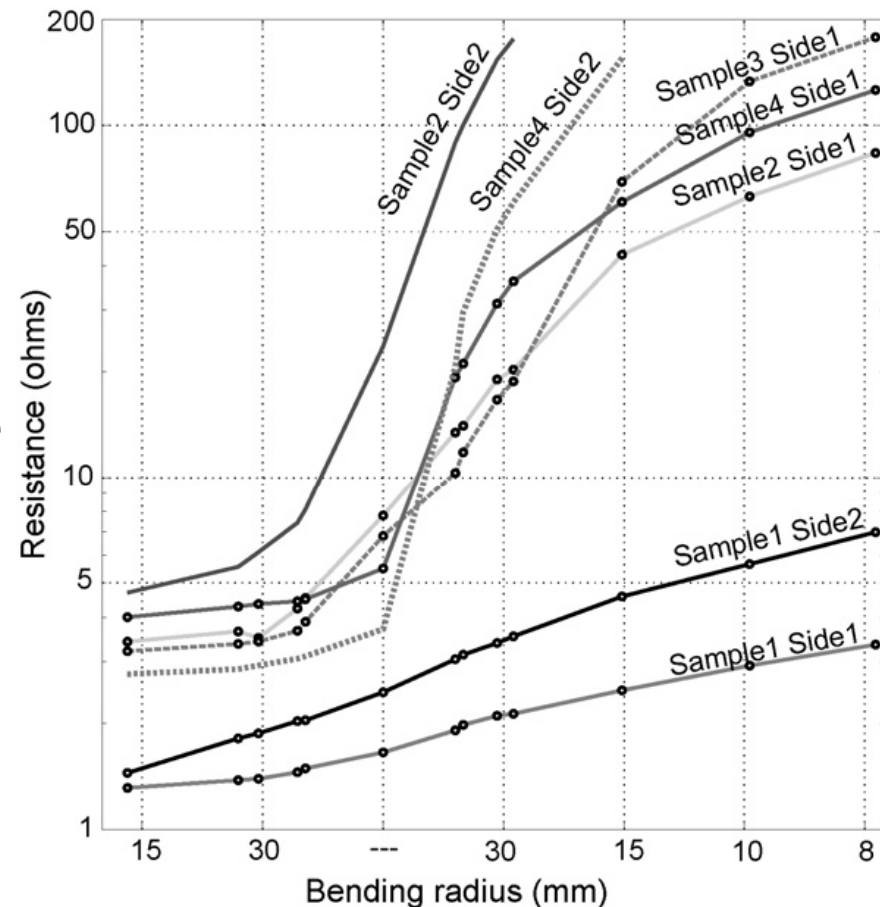
- **Concentration graph**



– Bending related to concentration → electric properties

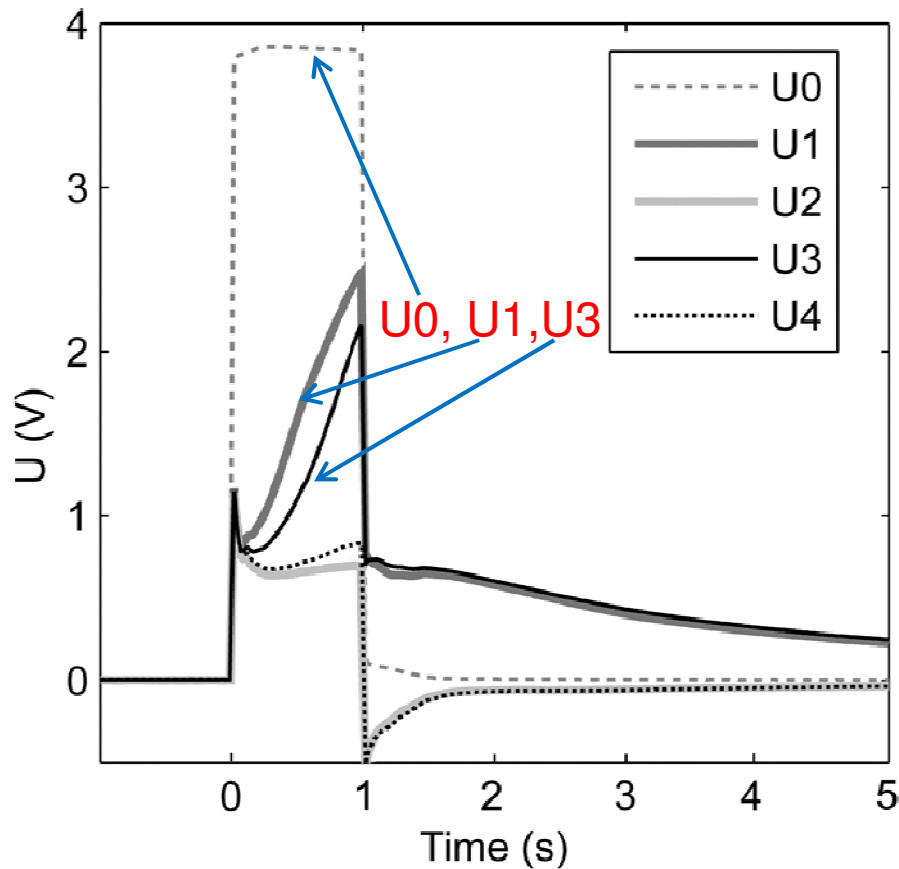
Electrode modeling - Motivation

- 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



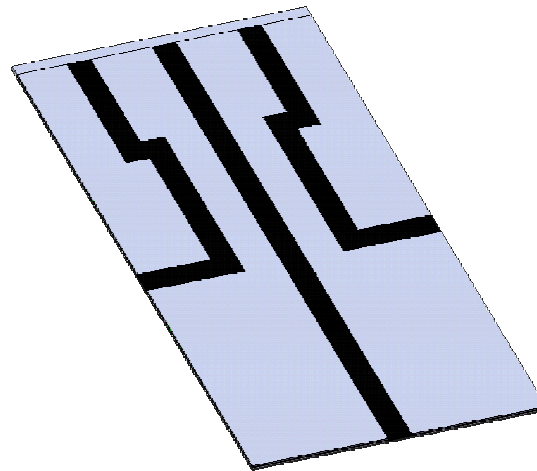
- ... which leads to a voltage drop along the electrode
 - U_0 , U_1 , U_3 measured on the one side of IPMC
 - Some of the drop is due to electrolysis
 - Part of it is due to surface resistance

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

Electrode modeling - motivation

2) Patterned electrodes

- 3D bending
- Different areas with different surface characteristics



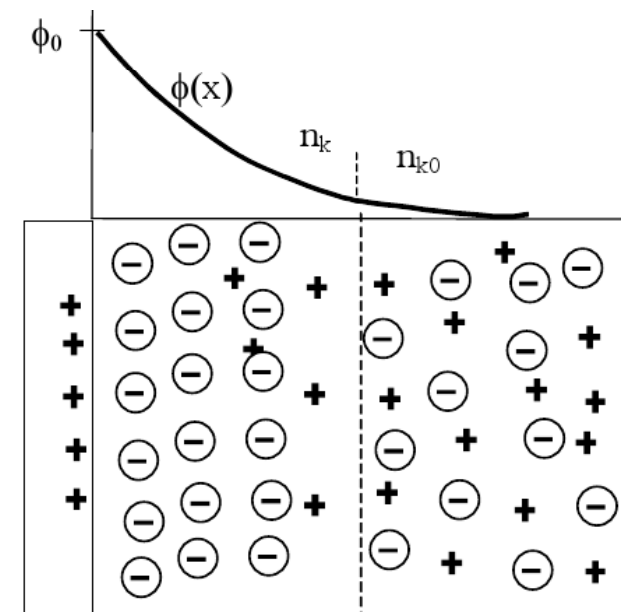
3) Electrode conductivity characterization

Surface resistance model - background

- Tie together the current flowing through the surface and the ionic current inside the polymer
- Ramo-Shockley theorem
 - Plasma physics *
 - 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:**

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

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

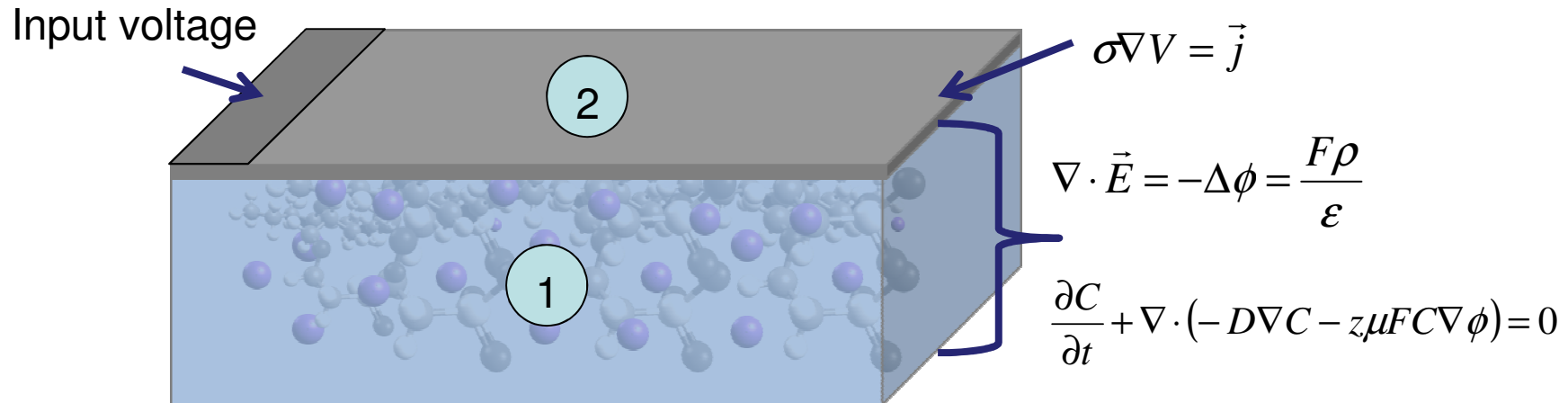
$$\vec{J} = \frac{F}{d} \int_0^d \vec{f} \cdot \vec{dy} \quad \longleftarrow \quad \begin{array}{l} \text{Final form that is} \\ \text{used in the} \\ \text{simulations} \end{array}$$

Surface resistance model - Comsol

- **Implementation in Comsol**

- **2 different domains are modeled**

- 1: Polymer (Nernst-Planck and Poisson' equation)
- 2: Electrode (Ohm' law)

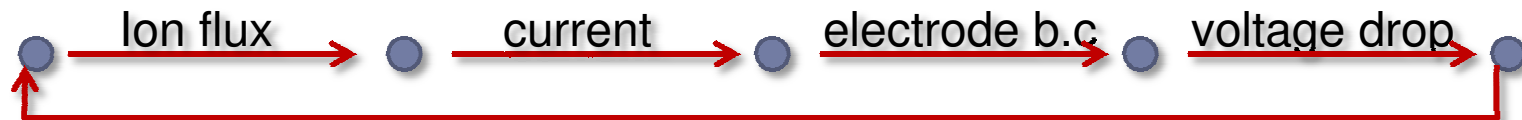


- **B.C. Boundary between the bulk Nafion and electrode:**

- 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

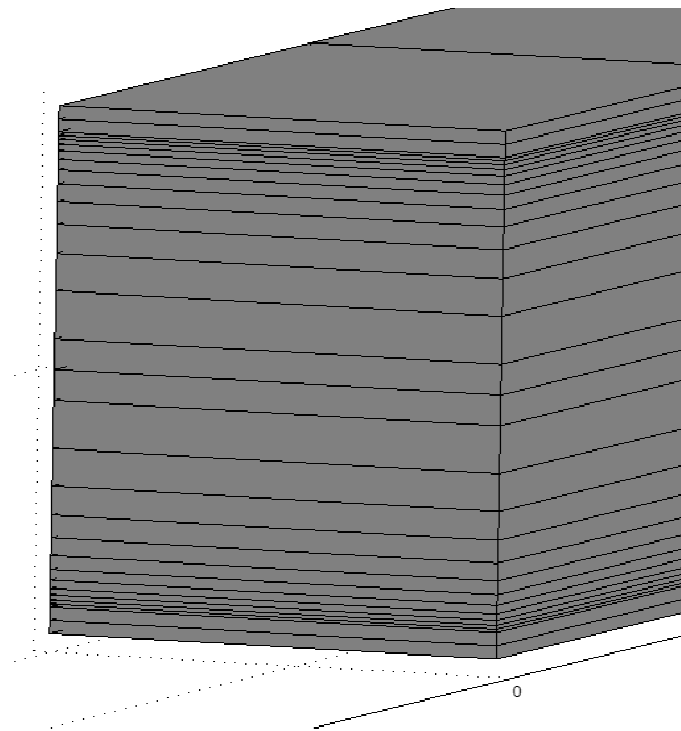


- The voltage of the electrode model, in turn, becomes a boundary condition to the Poisson equation, which is responsible for the ion flux

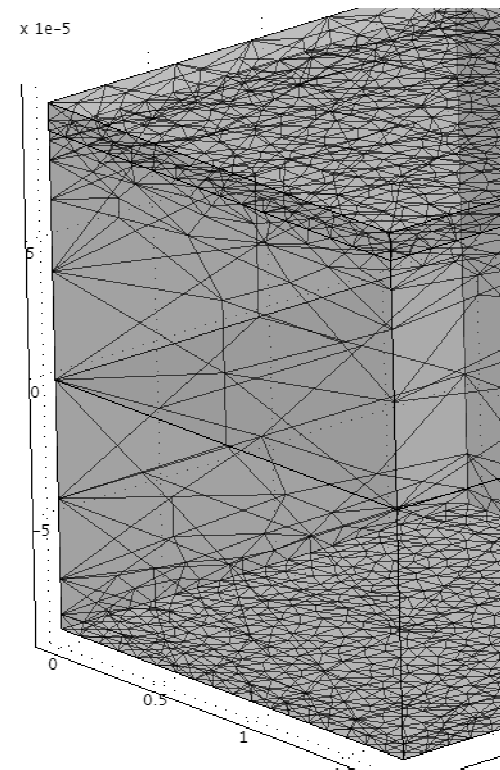
Surface resistance model - Comsol

- Implementing in Comsol – meshing

Regular mapped mesh - faster

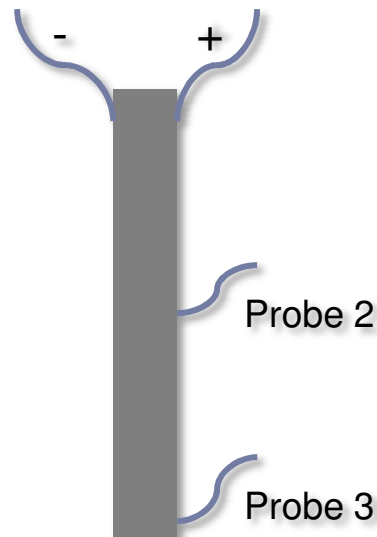
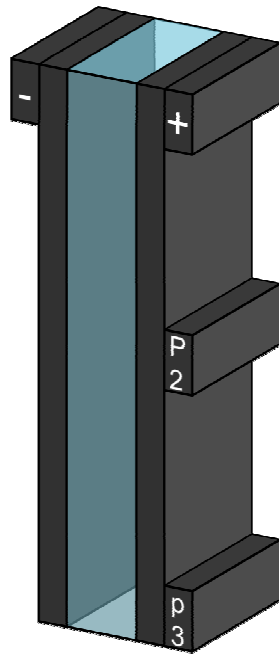


Free mesh – due to projection coupling
(both for 2D and 3D simulations)

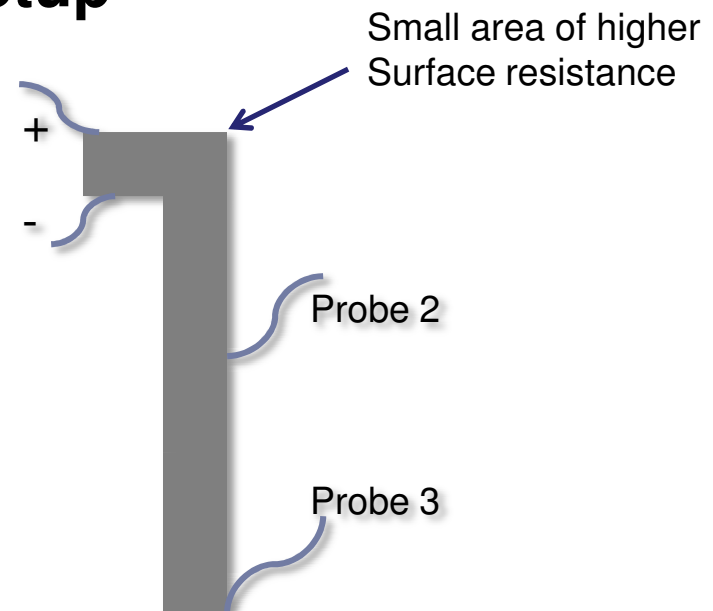


Results

- 2D modeling – experimental setup



Straight IPMC



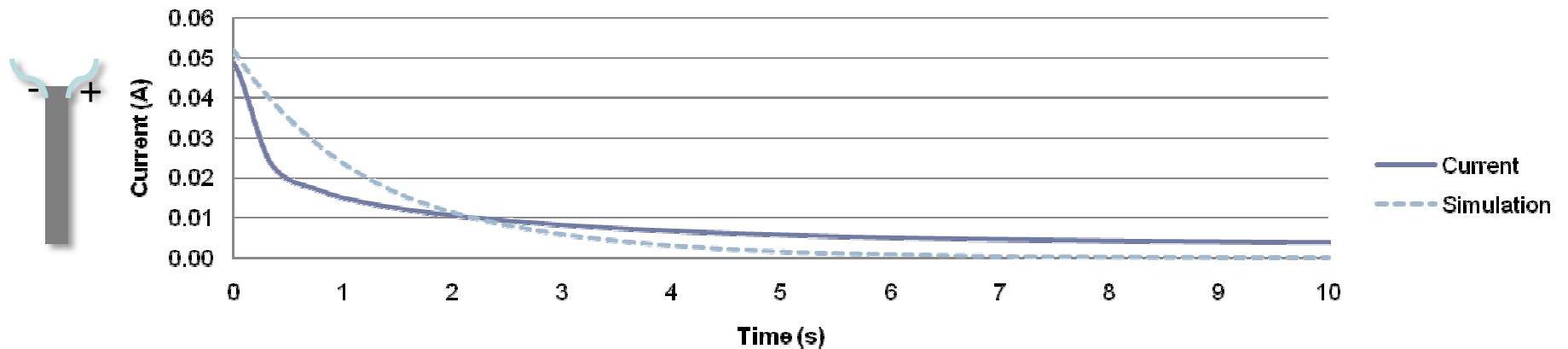
Bent IPMC

- 2D modeling – the model

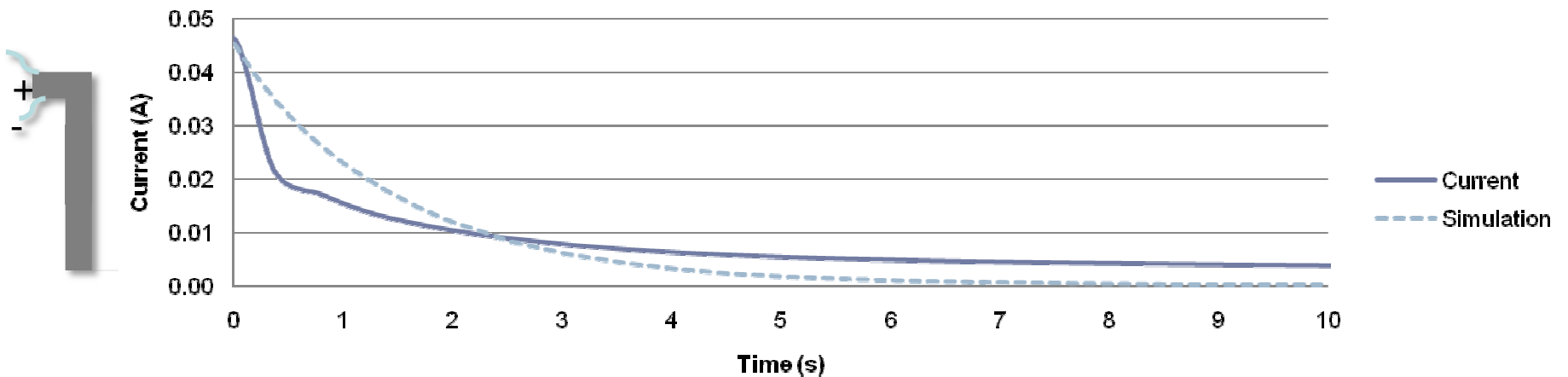


Results – 2D model, current

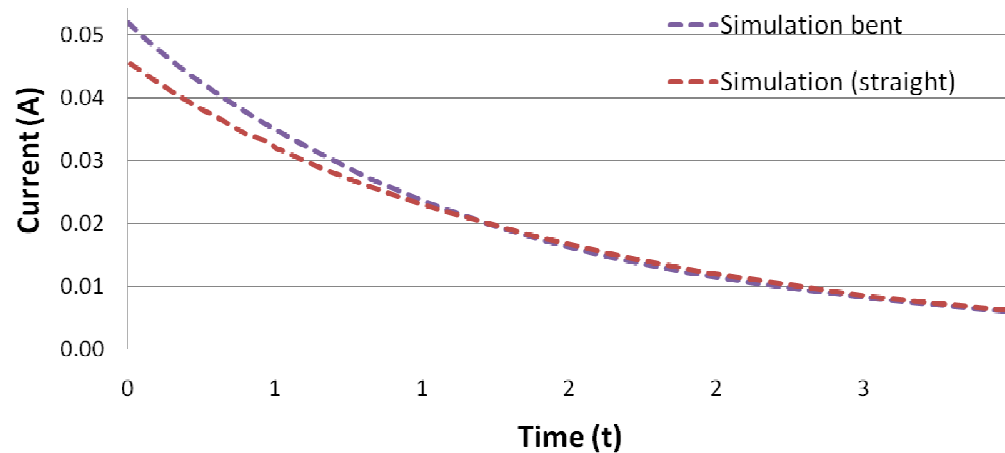
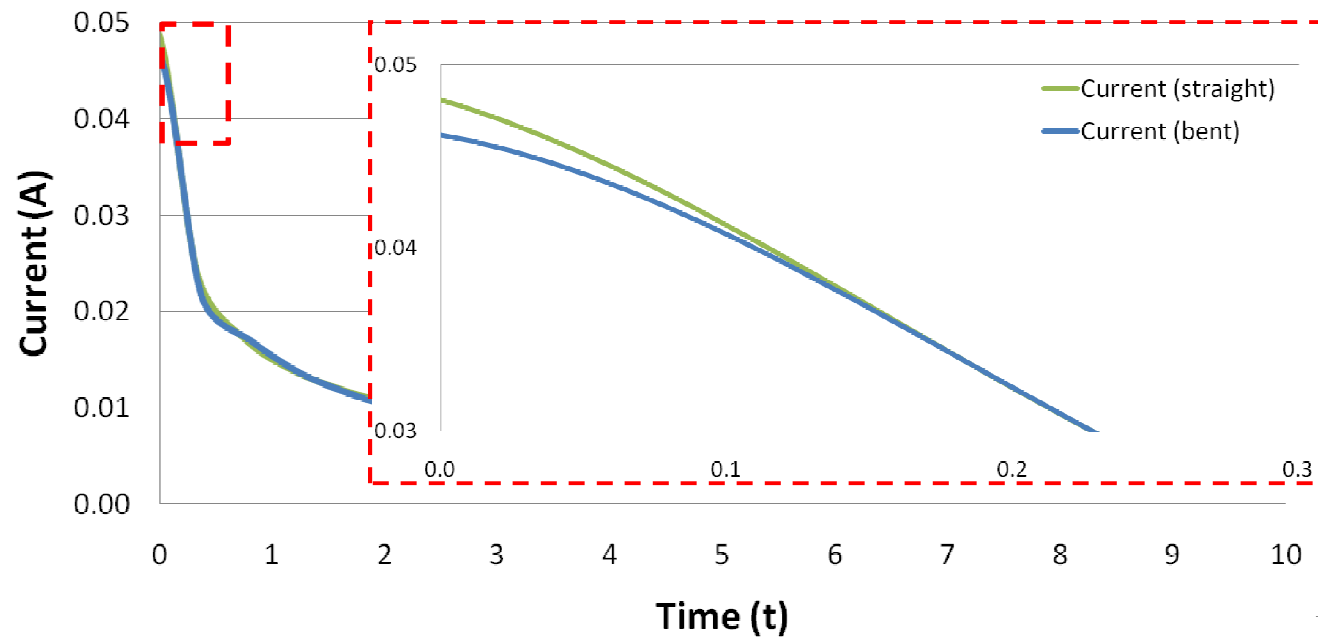
Current (straighth)



Current (bent)

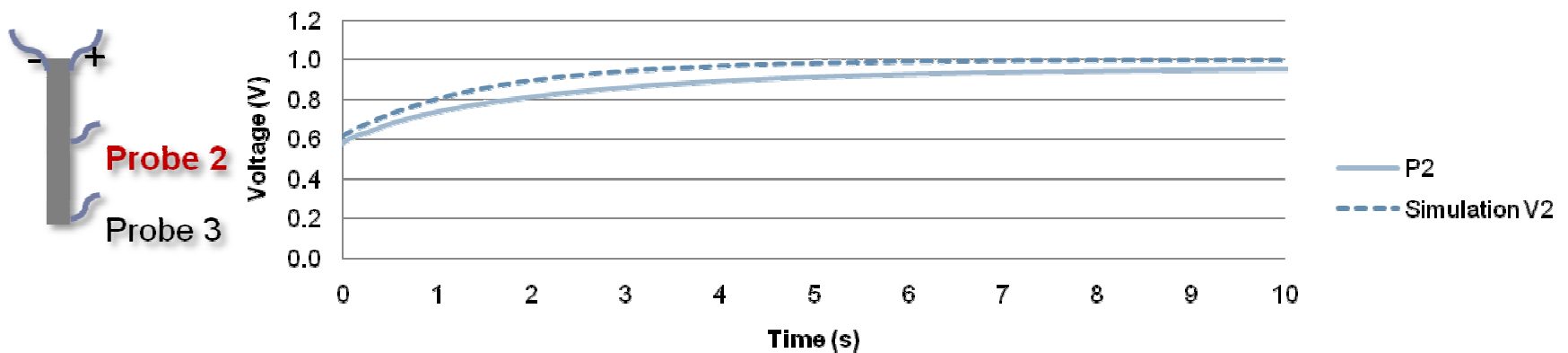


Results – 2D model, current

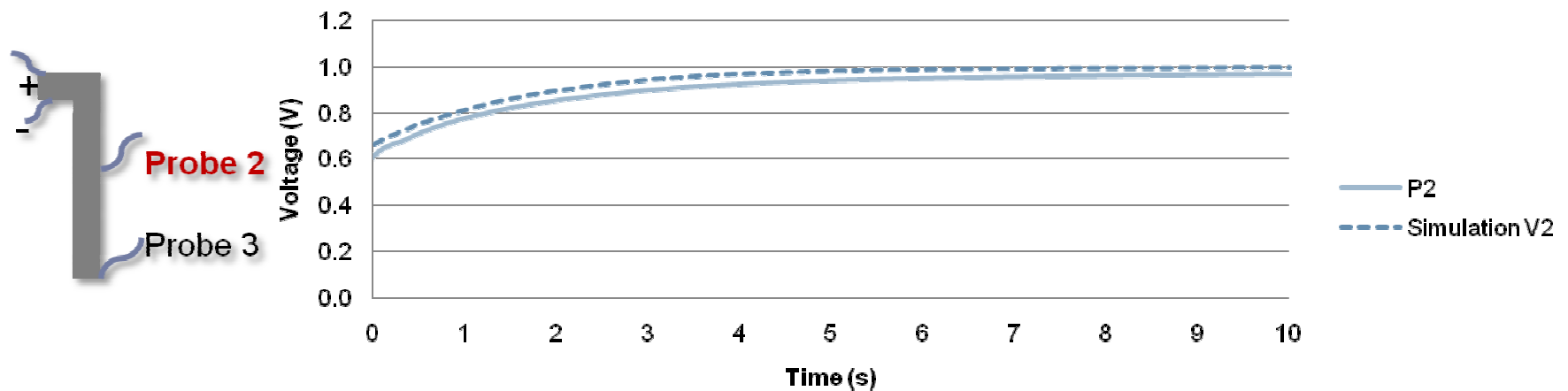


Results – 2D model, Voltage

Voltage (middle probe)

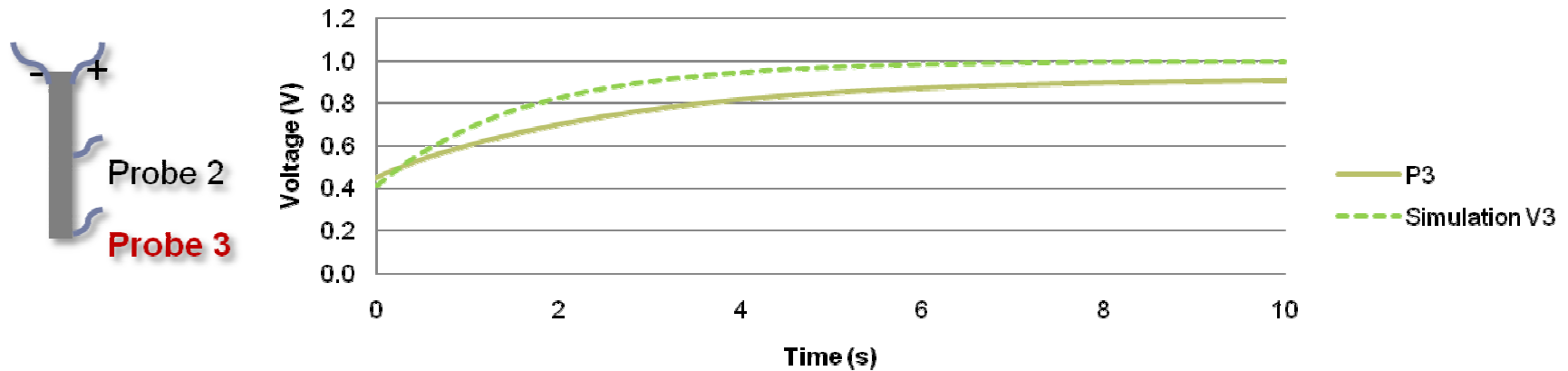


Voltages (bent, middle probe)

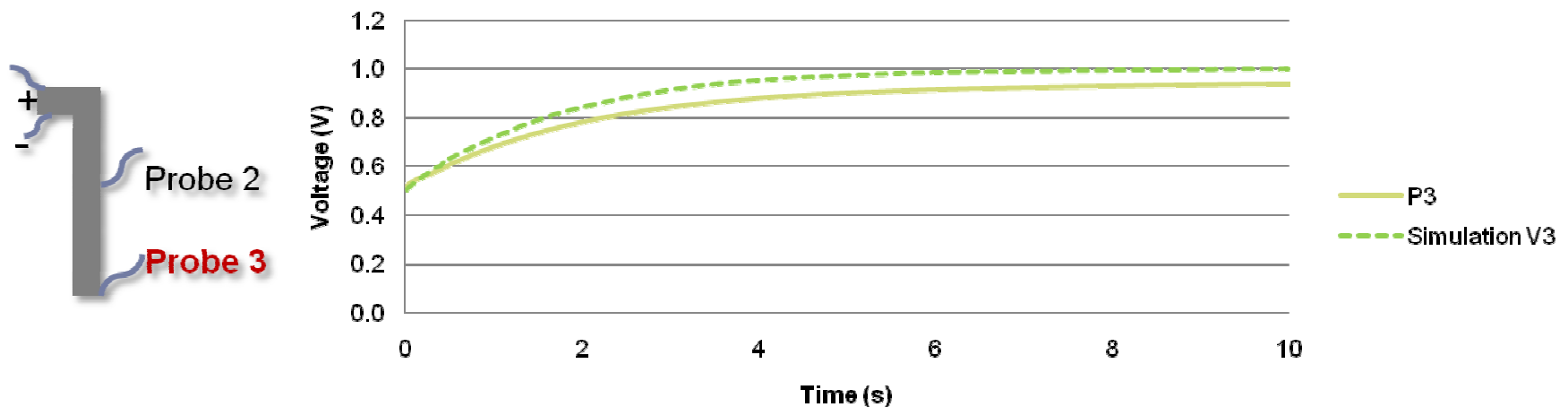


Results – 2D model, Voltage

Voltage (end probe)



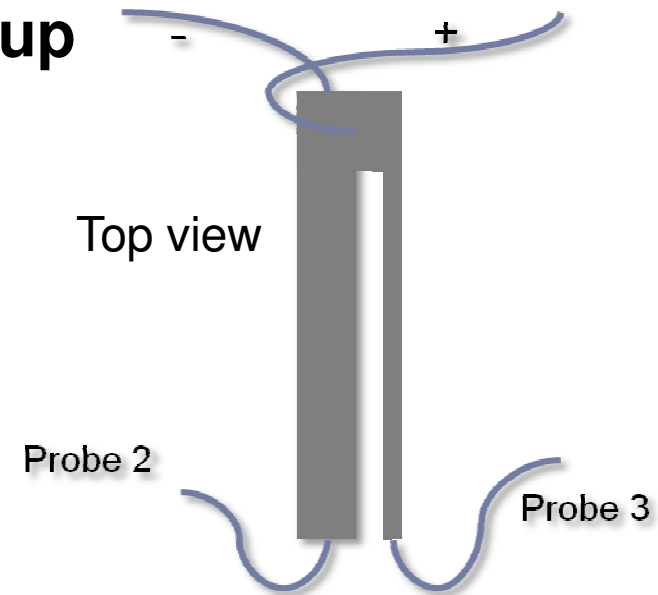
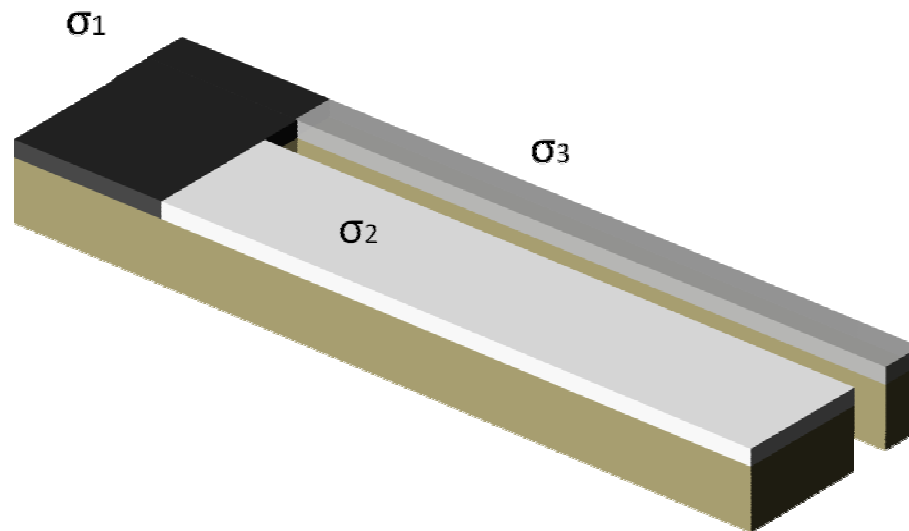
Voltages (bent, end probe)



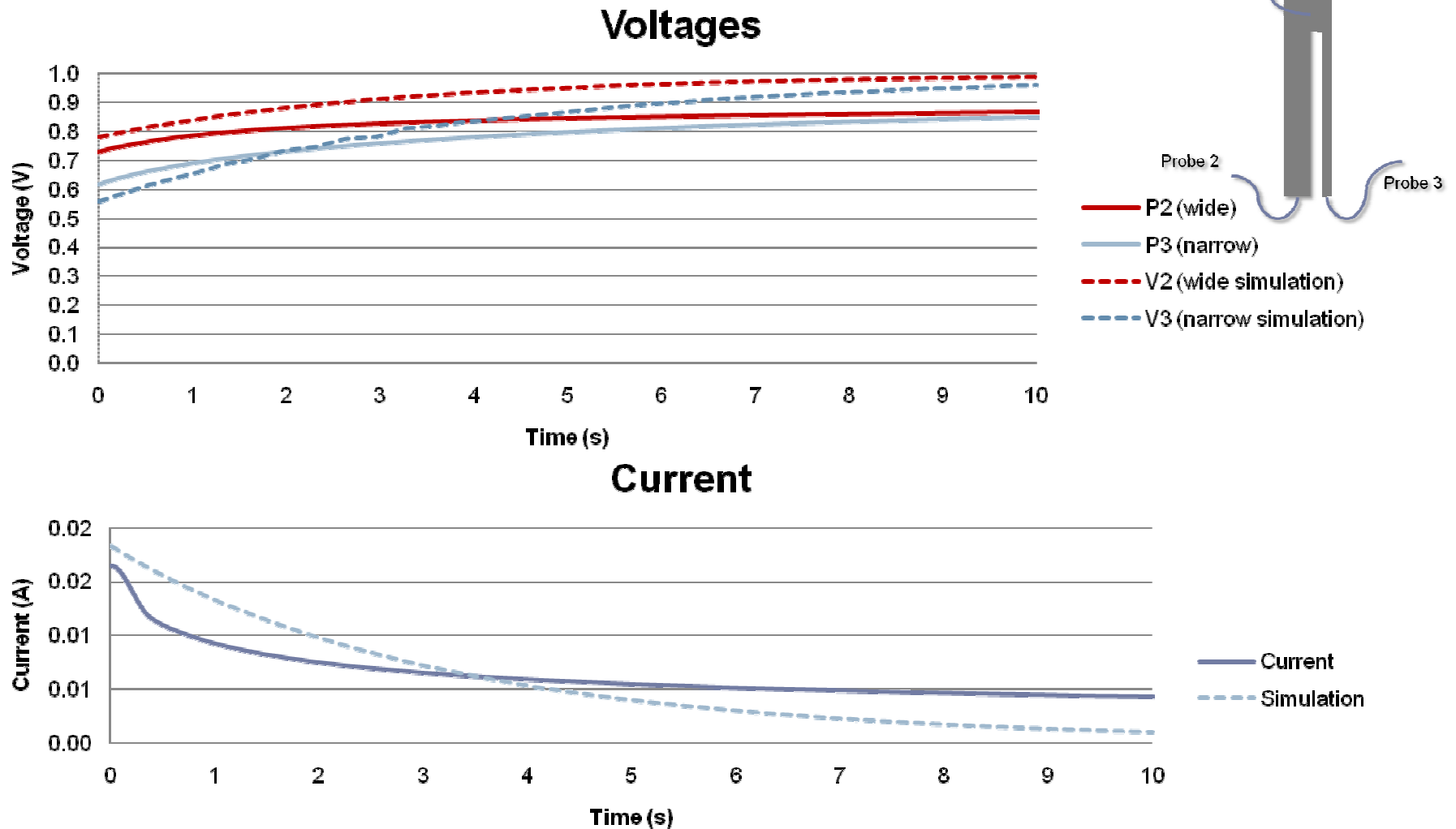
Results

- 3D modeling – experimental setup

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



Results – 3D model

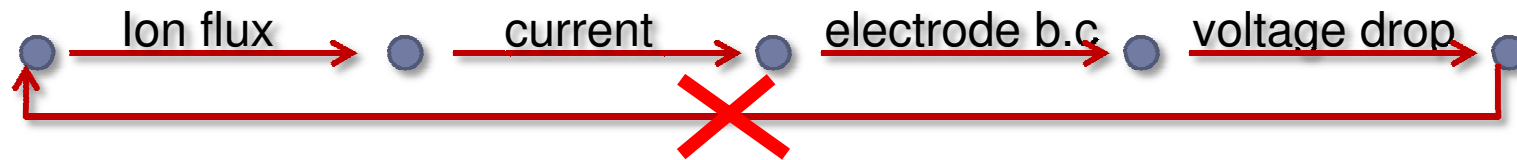


Discussion

- **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

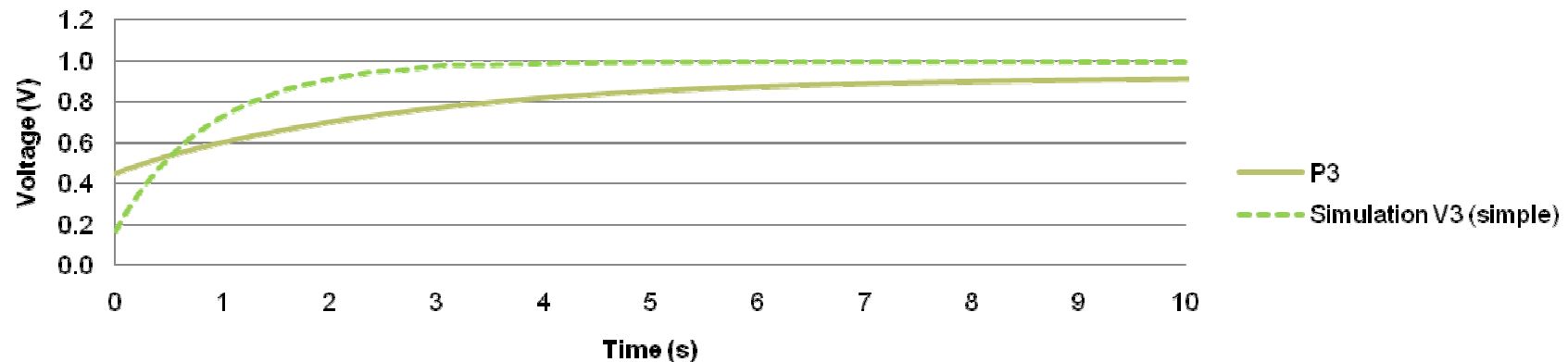
- **Loose the feedback**



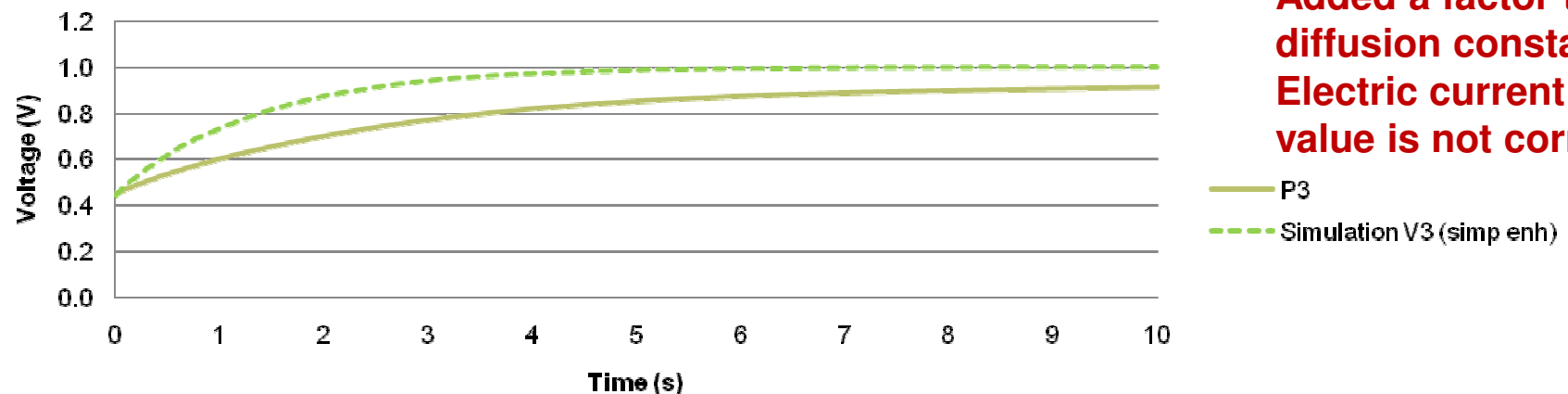
- Better convergence
- Reduced calculation time
- Ionic current does cause the voltage drop on the electrodes
- The voltage drop does not change the ionic current
- Could be used for characterizing the surface – does not change the ionic behavior

Results – simplified model

Voltage (end probe - simp)



Voltage (end probe - simp enhanced)



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

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

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



Thank you

- Questions?

