Finite element simulations of the bendiong of an IPMC sheet

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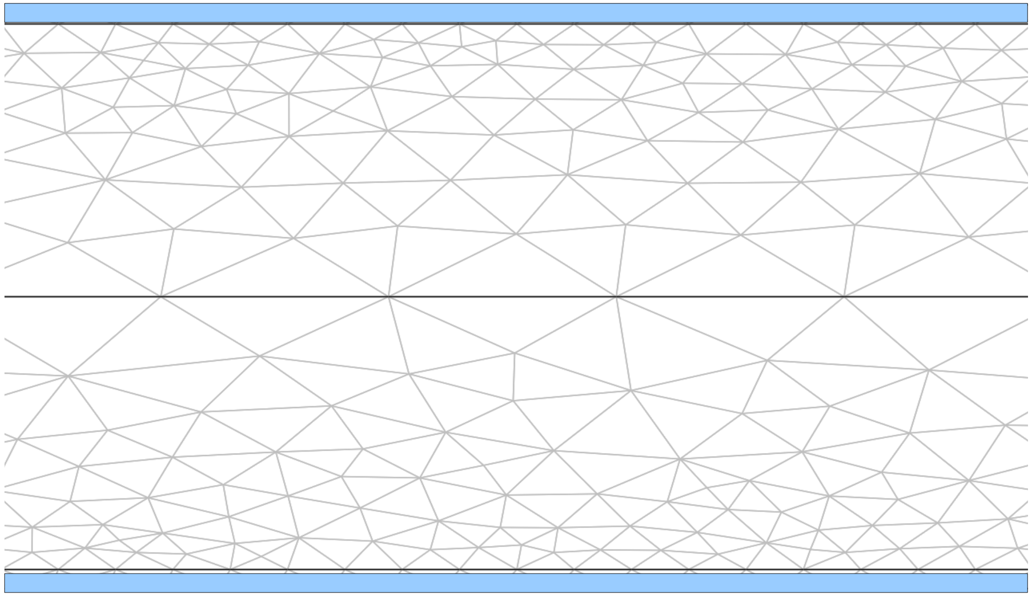
Background

- IPMC – ionic polymer-metal composites are highly porous polymer materials, such as Nafion, filled with some kind of ionic conductive liquid
- The sheet of polymer material is coated with a thin metal layer – usually platinum or gold
- In electric field, freely movable ions inside the polymer migrate towards an electrode, causing expansion of material at the one end and contraction at the other end

- FEM – Finite Element Method
  - Used as a technic of modeling in this work

Introduction

- The goal: Time dependent FEM model for an IPMC
- Domains to be considered
  - Mechanical
  - Electrostatic
  - Mass transfer
- The designed model is 2D
- Adding more complexity – electrochemical reactions

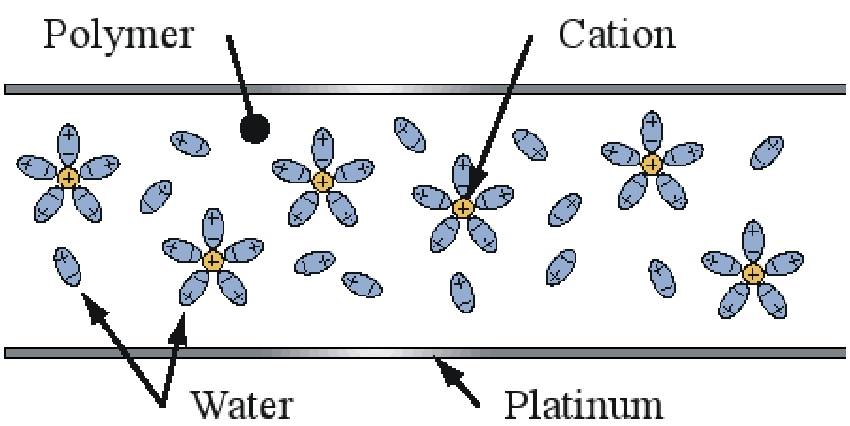


Simulations – cation migration

- Nernst-Planck equation
  - Diffusion
  - Migration
  - Convection

$$\frac{\partial C_i}{\partial t} + \nabla \cdot (-D_i \nabla C_i - z_i \mu_i C_i \nabla \phi) = -\vec{u}_i \cdot \nabla C_i$$

- Voltage causes migration of cations towards cathode
  - That's also the cause of the current in the circuit
- All anions are fixed to the polymer backbone



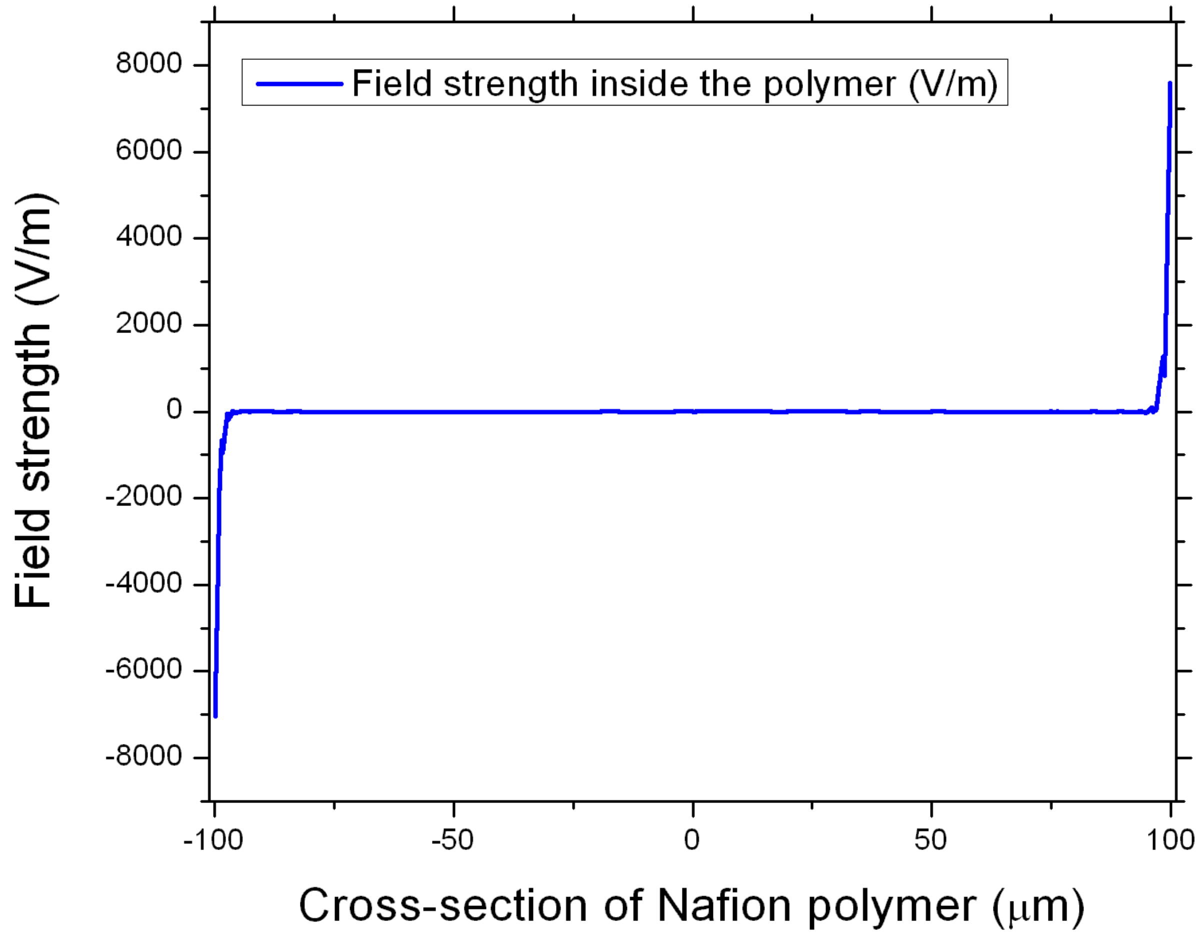
Simulations – cation migration (2)

- Charge imbalance inside the IPMC results in electric field
  - opposite to the applied field
- Gauss' law:

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

- Steady state of cations – when the generated field cancels out applied field.

Simulations – cation migration (3)



Actuation of an IPMC

- FEM model – a bit different approach
  - Euler beam model is not used
  - Our model is dynamic, not static
  - Viscoelasticity

- Assumption – charge imbalance creates longitudinal force inside the IPMC

$$\vec{F} = (A \cdot \rho + sgn(\rho) \cdot B \cdot \rho^2) \cdot \hat{x}$$

- We consider two terms – density and square of density
- Constants A and B are fitted using experimental results

Mathematics behind the bending

- Continuum mechanics equations have been used
- The stress is related to force in each point of the polymer:

$$-\nabla \cdot \sigma = \vec{F}$$

- The stress is related to strain:

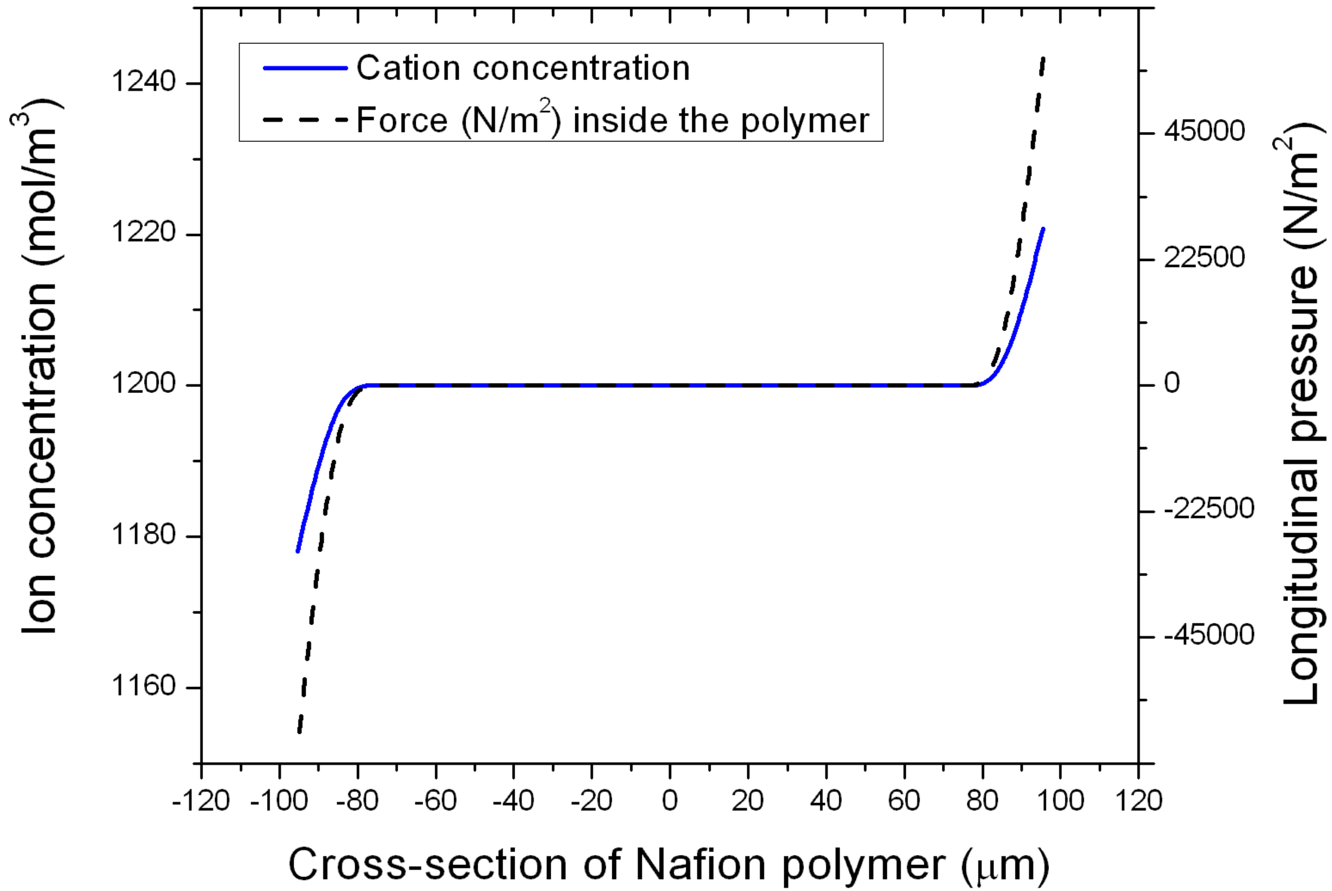
$$\sigma = D\,\varepsilon$$

where ε and σ are column vectors with dimensions of 6

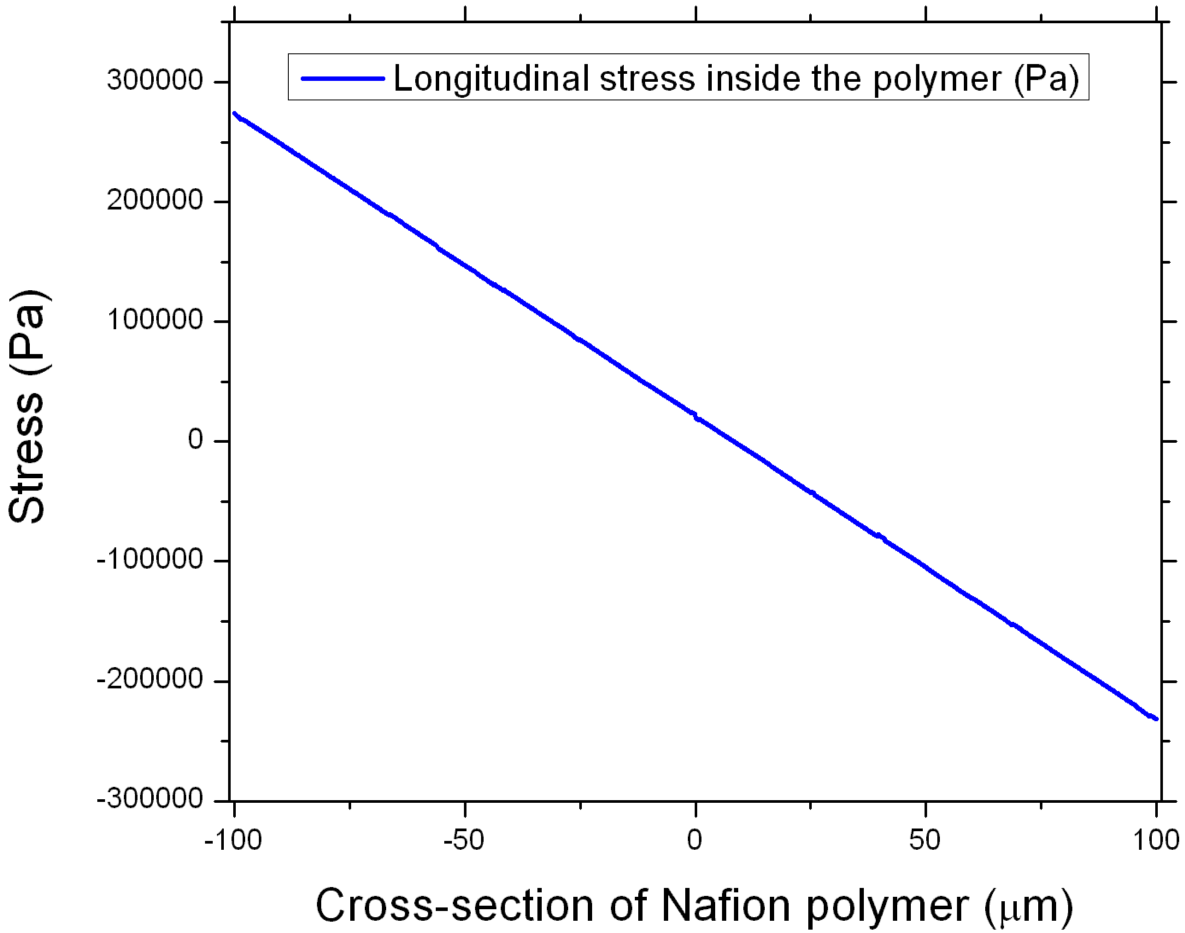
- Finally, the strain is related to displacement:

$$\varepsilon_i = \frac{\partial u_i}{\partial x_i},\ \varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i}\right)$$

Simulations – cation migration, force



Simulations – generated stress



Transient analysis of bending

- Time dependent equations -> dynamic problem
- Motion of an IPMC sheet is described

$$\rho \frac{\partial^2 \vec{u}}{\partial t^2} - \nabla \cdot c \nabla \vec{u} = \vec{F}$$

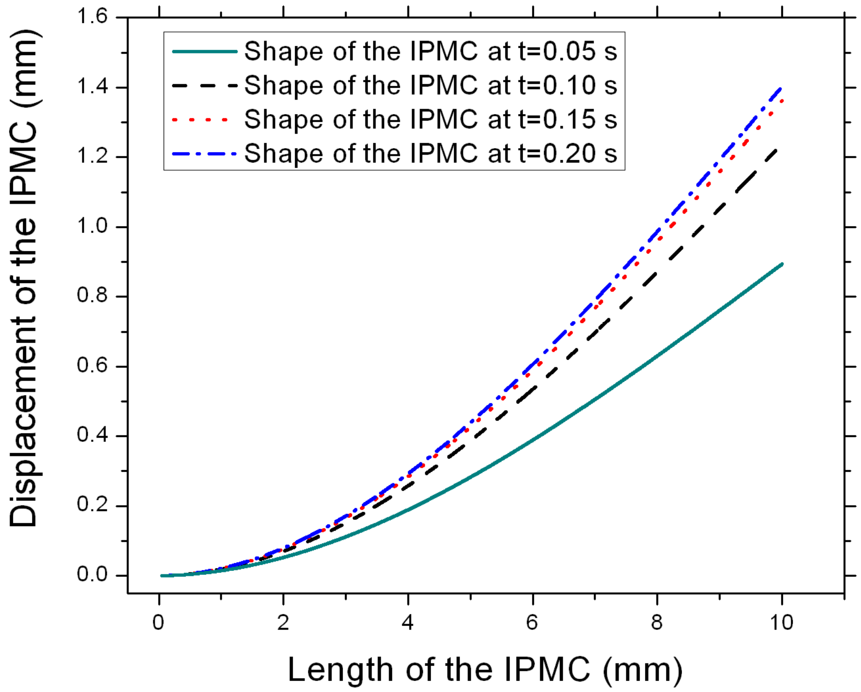
- Rayleigh damping model:

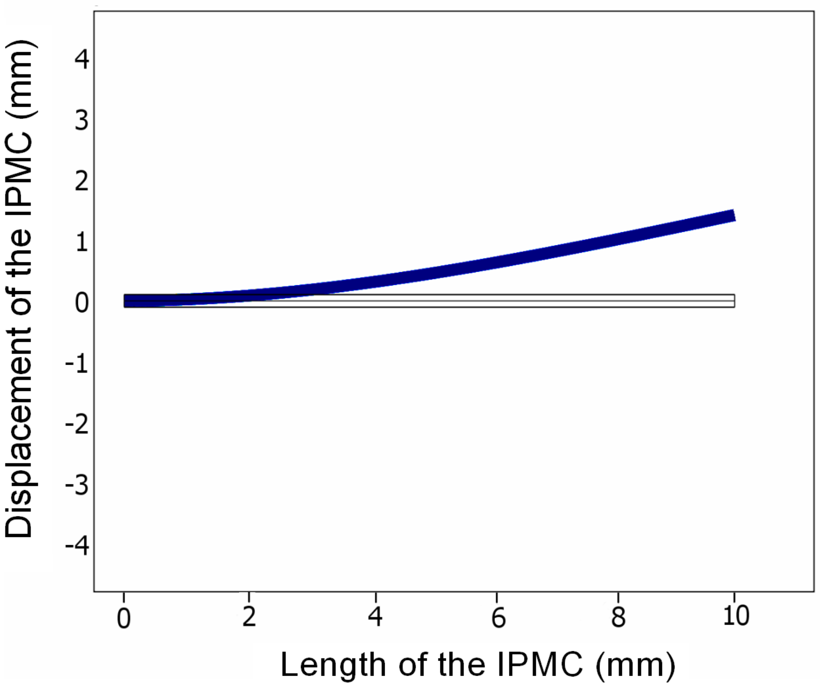
$$m \frac{d^2 u}{dt^2} + \xi \frac{du}{dt} + ku = f(t) \qquad \xi = \alpha m + \beta k$$

- ξ is a damping parameter. m is mass and k is stiffness. By coupling those equations for the system of multiple degrees of freedom:

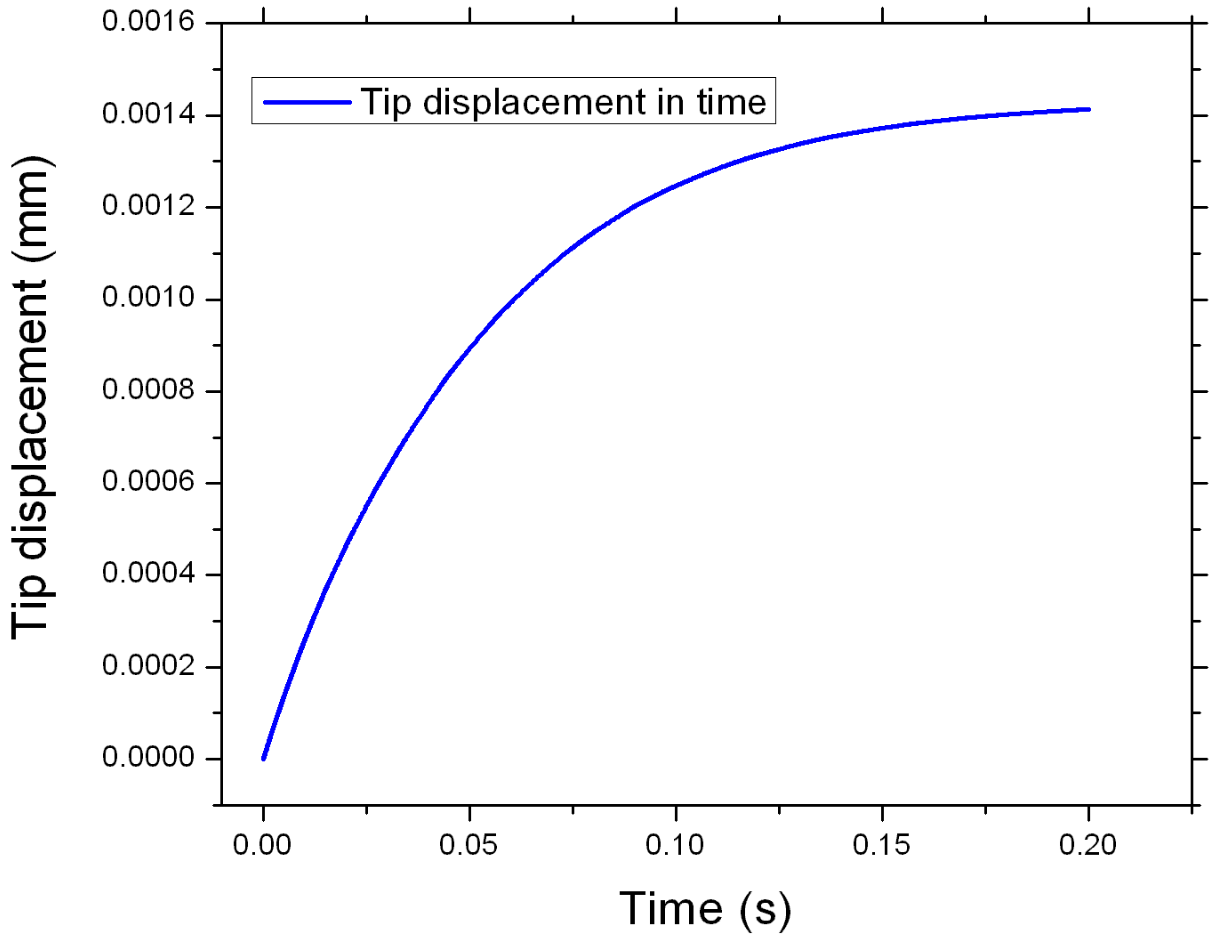
$$\rho \frac{\partial^2 \vec{u}}{\partial t^2} - \nabla \cdot [c \nabla \vec{u} + c \beta \nabla \frac{\partial \vec{u}}{\partial t}] + \alpha \rho \frac{\partial \vec{u}}{\partial t} = \vec{F}$$

Simulation results





Tip displacement in time



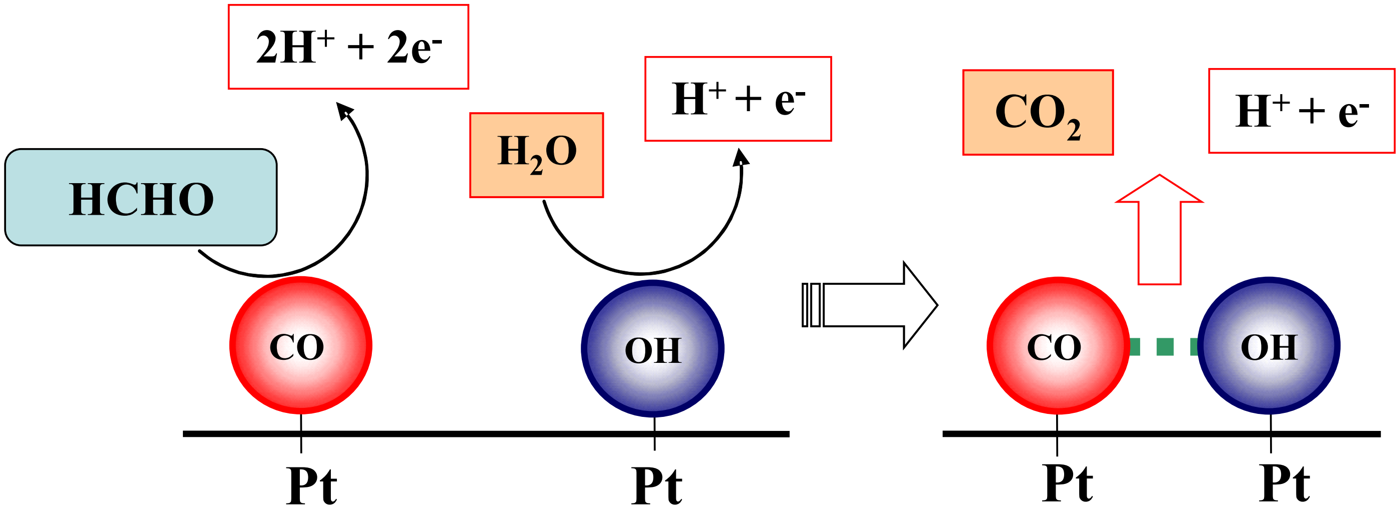
Conclusions

- We have a Finite Element model, which describes...
  - the movement of ions inside the polymer
  - the electric field
  - the dynamic bending of an IPMC sheet
- For next, we add some complexity – electrochemical oscillations

Self-oscillations

- Electrochemical oscillations – common phenomena in nature
- Oscillations have also been experimentally studied
- Tests with IPMC:
  - immersed into acidic formaldehyde (HCHO) solution
  - applied constant voltage 0.75V
  - result: current oscillations and oscillating bending

- Cause of the oscillations are electrochemical reactions on Pt surface



Simulating self-oscillations

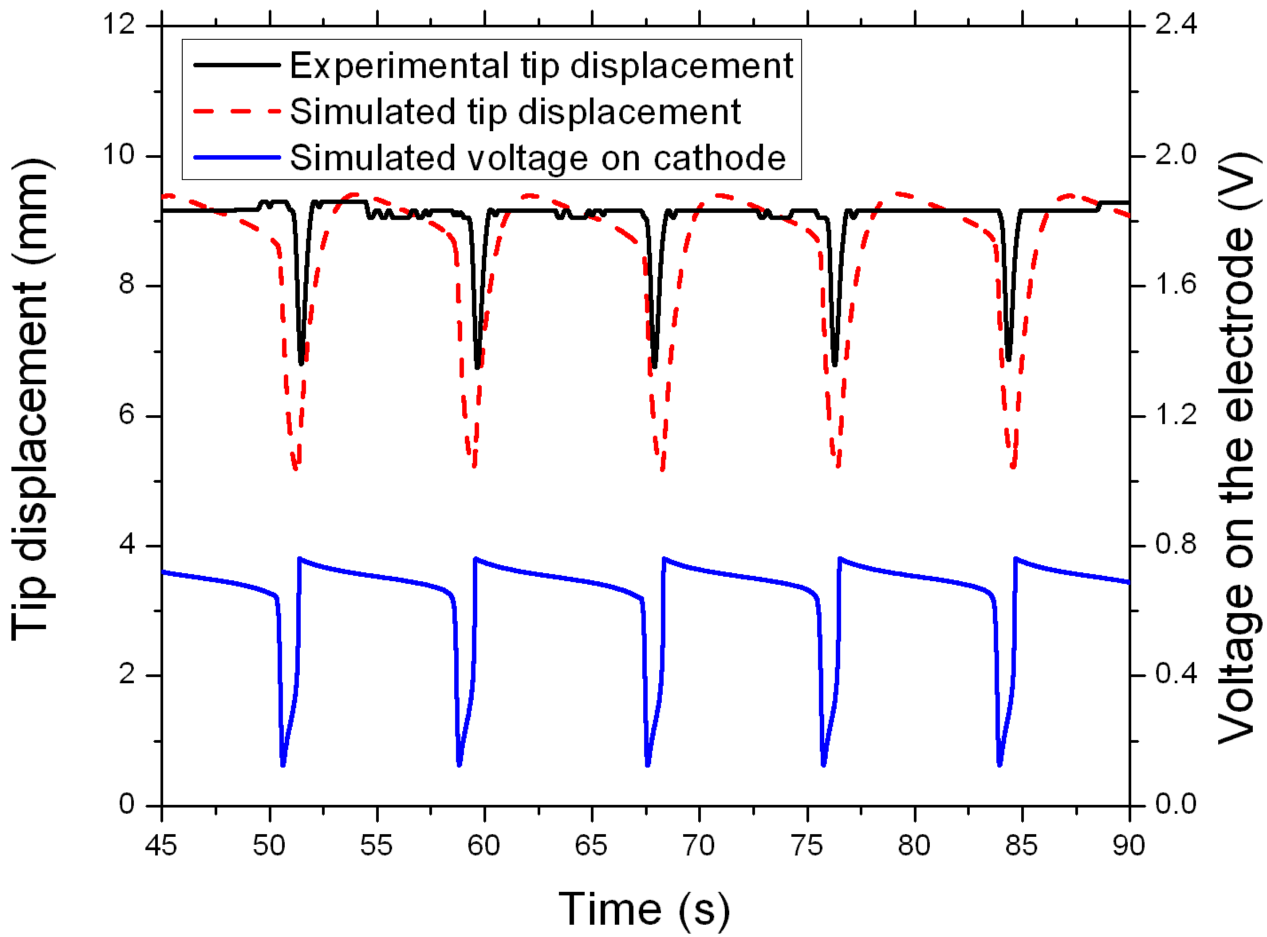
- A double layer were initialized near the platinum surface.
- On that suface, the following reaction is modeled:

$$HCHO + * -> Pt - CHO_{ads} + H^{+} + e^{-}$$

- 4 dynamic variables must be modeled on the platinum surface
  - time dependence of adsorption coverage of CO
  - time dependence of adsoprtion coverage of OH
  - HCHO concentration change in double layer
  - time dependence of potential on cathode

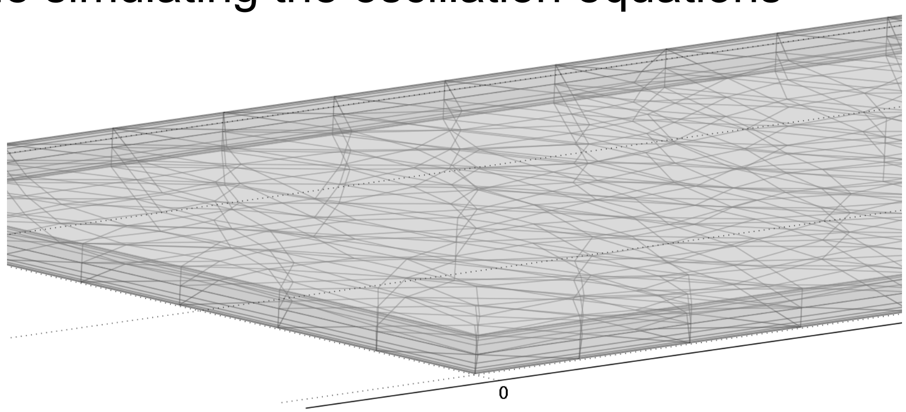
- These equations were coupled to the basic model...

Self-oscillations – model and experiment



Conclusions and future plans

- 2D, basic FEM model was developed to describe time dependent actuation of an IPMC muscle
- In addition, more complexity was added by coupling a problem of electrochemistry.
- Also experimental and simulatios results were compared and quite good agreement were found
- For future:
  - Adding 3rd dimension to the model
  - Considering fluid viscosity and corresponding equations inside the polymer
  - Work on the simulating the oscillation equations



Questions

Thank you for your attention!