Research review

My research at the moment (12/01/06)

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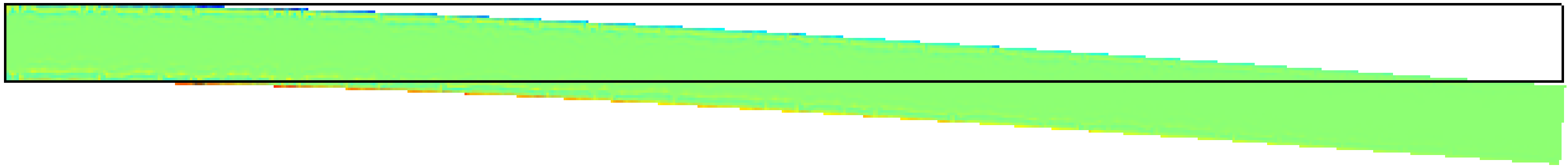
Previously completed tasks

- Model of movement of the cations.
  - $\frac{\partial C}{\partial t} + \nabla \cdot (-D \nabla C - zuC \nabla V) = 0$
- Model of electric field change due to the ion movement
  - $\nabla^2 \phi = -\rho$



Bending model

- Assumption is that internal forces are due to charge imbalance
- No Euler beam theory
- Plane strain module, in Comsol, instead:
  - More suitable for finite element analysis
  - Dynamic instead of static solution.

Bending model - overview

- Body forces in are defined as

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

- Where σ is symmetric stress tensor and it is related to strain in the following way: $\sigma = D\varepsilon$
  - Where again

$$\varepsilon = \begin{bmatrix} \epsilon_x & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{xy} & \epsilon_y & \epsilon_{yz} \\ \epsilon_{xz} & \epsilon_{yz} & \epsilon_z \end{bmatrix} \quad \epsilon_i = \frac{\partial u_i}{\partial x_i} \quad \epsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

  - And D is elacticity matrix (inverse D is flexibility matrix). Includes variables such as *Poisson's ratio* and *Young's modulus*

Bending model – Rayleigh damping

- For transient analysis, we also have to consider damping!
- Comsol uses Rayleigh damping. Motion of the system:

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

$$\xi=\alpha m+\beta k$$

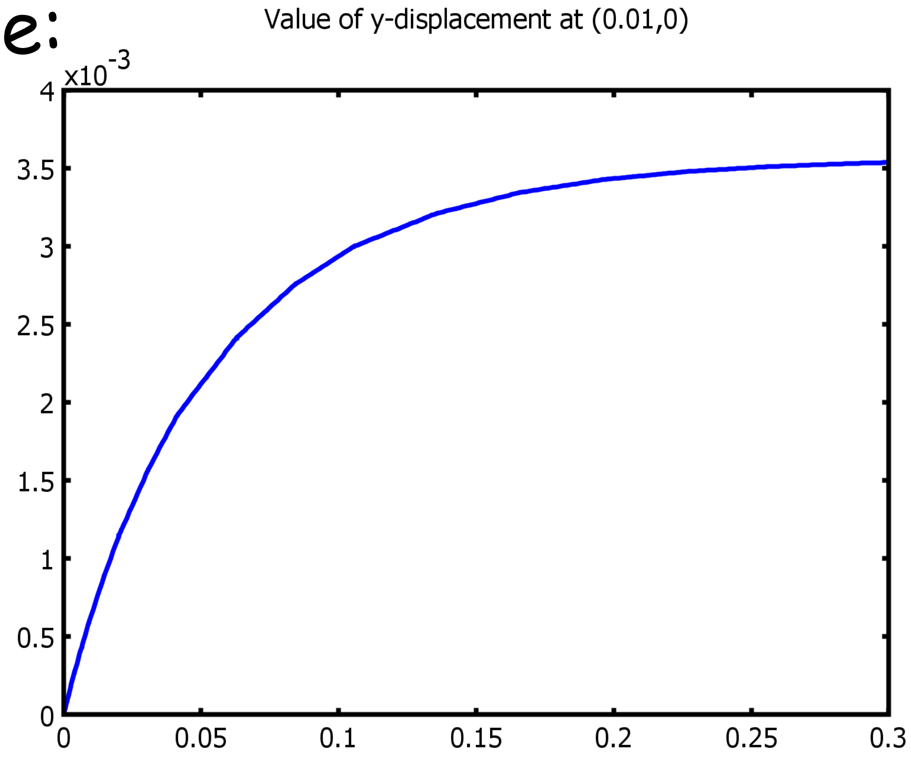
  - So the damping parameter ξ is expressed in terms of mass m and stiffness k
    - In my model: $\alpha=1\left[\frac{1}{s}\right],\beta=0.05[s]$

Bending model - forces

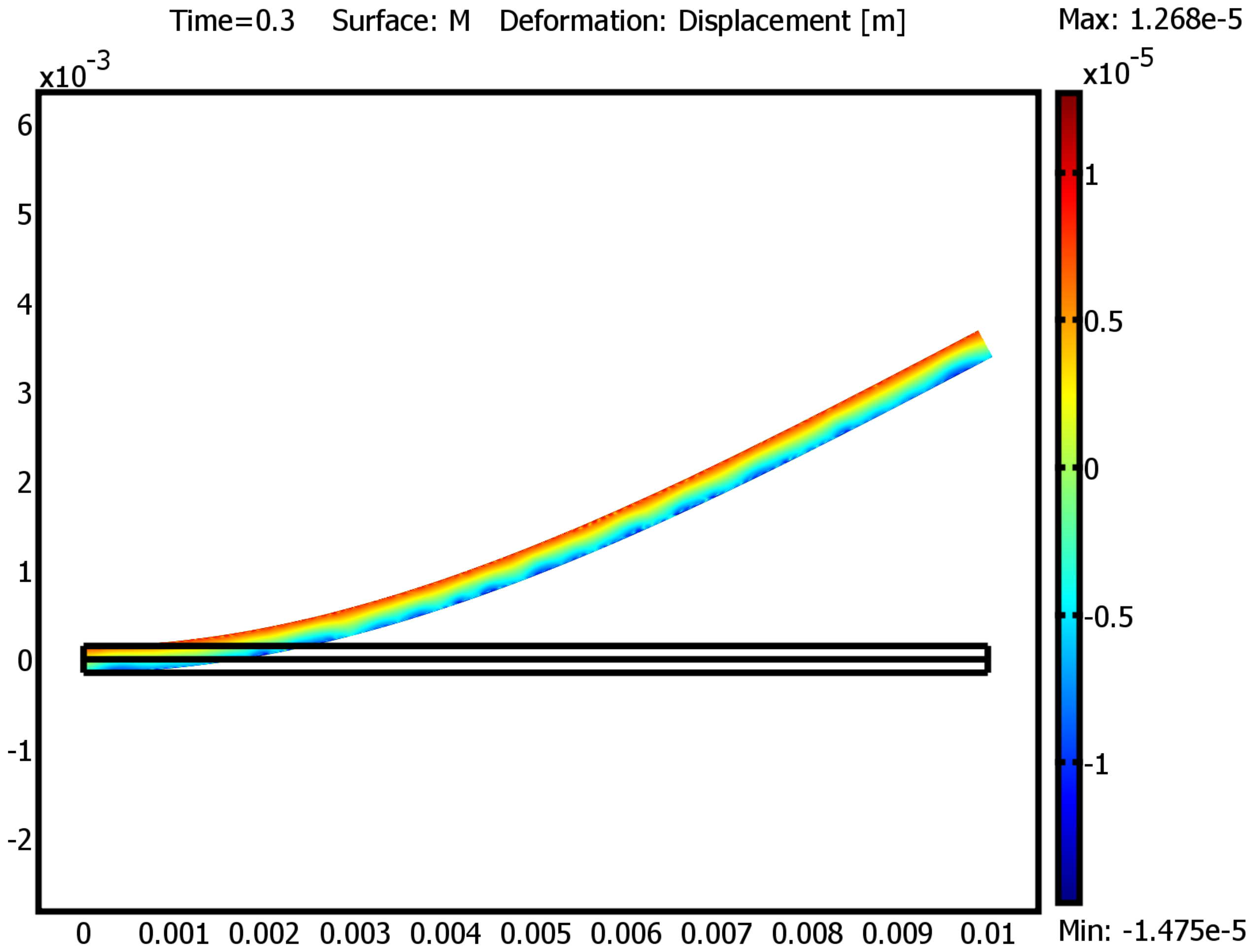
- Force in each point of IPMC is defined as:

$$A \cdot (c_{Na} - c_{SO})$$

- Displacement in time:



Bending model – an illustration

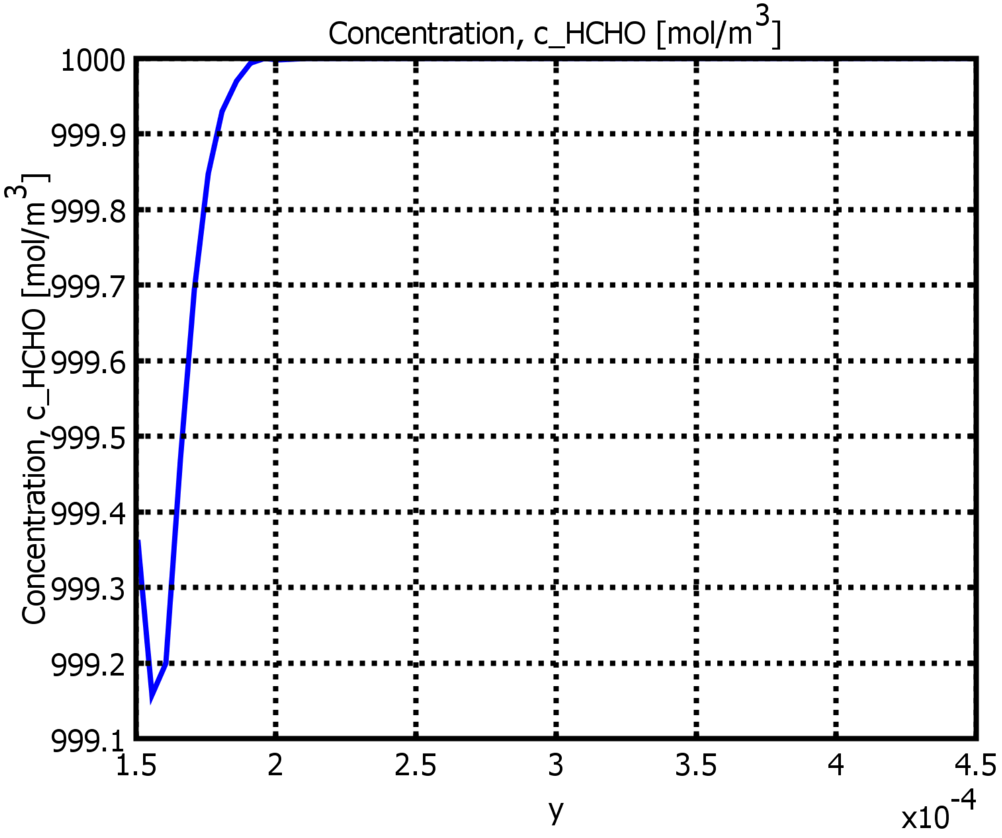


Electrochemical oscillation

- Electrochemical oscillations occur due to poisoning of Pt surface with CO, OH
- HCHO – poisons the surface with CO.
- First, introducing the diffusion layer (for HCHO diffusion)
  - An article suggested thickness of the diffusion layer about 0.3mm
    - It means that if chemical reactions occur at the one end of the layer, then there is still const. concentration of reacting species at the other end.

Electrochemical oscillation – conc. change

- Concentration change near platinum sufrace due to electrochemical reactions – must be considered in model!



Equations – on surface of patinum electrode

- Basically, I use slight modification of equations from Doyeon's PhD thesis.

$$\dot{\theta}_{CO} = \boxed{R\cdot} k_2\cdot(1-\theta_{CO}-\theta_{OH}) - k_4\cdot\theta_{CO}\cdot\theta_{OH}$$

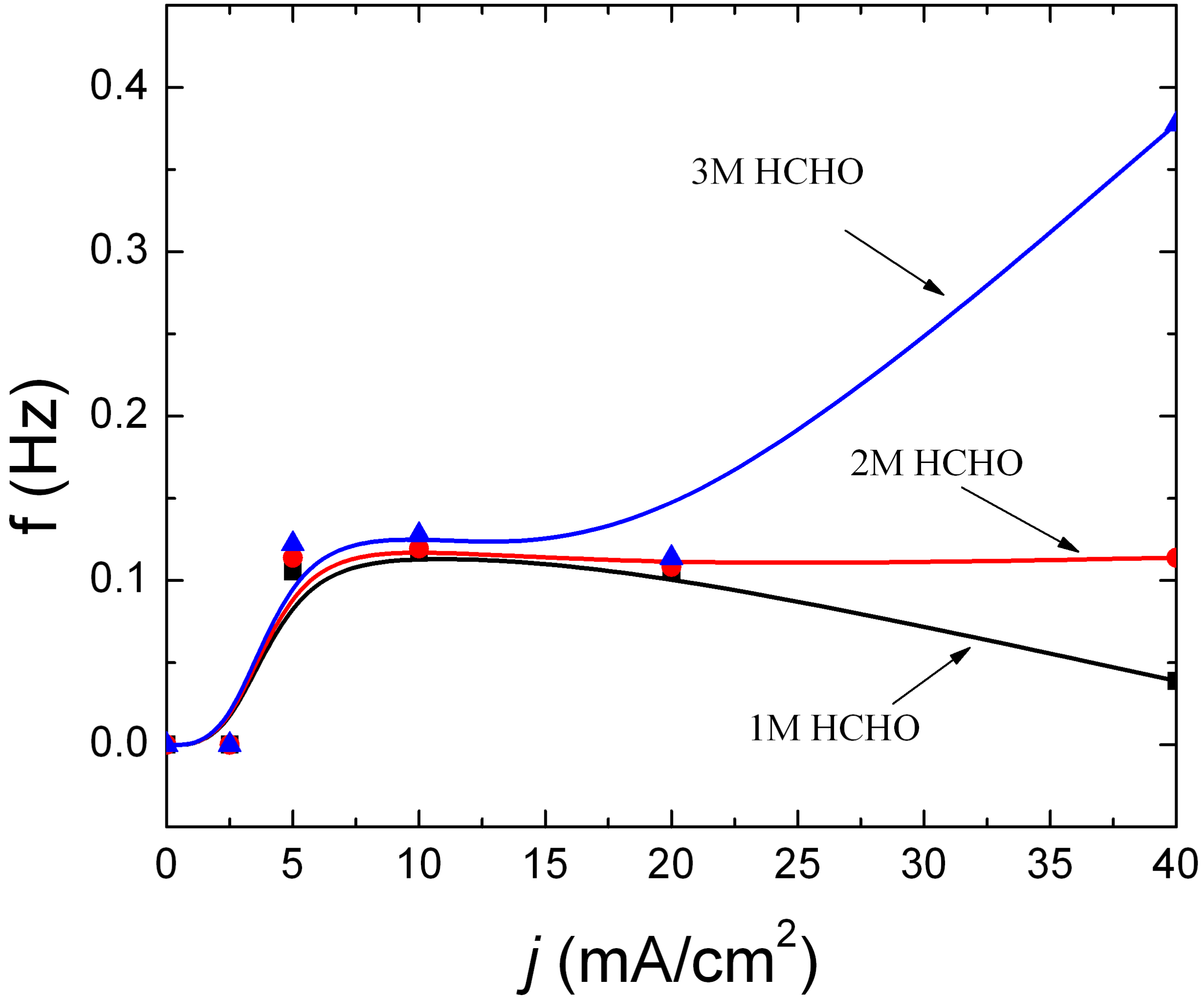
$$\dot{\theta}_{OH} = k_3\cdot(1-\theta_{CO}-\theta_{OH}) - k_3\cdot\theta_{OH} - k_4\cdot\theta_{CO}\cdot\theta_{OH}$$

$$\dot{E} = I_{th} + \boxed{(I-I_{th})\cdot R\cdot sgn(c_{HCHO}-c_{HCHO2M})} - j\cdot(k_1\cdot(1-\theta_{OH}-\theta_{CO}) + k_4\cdot\theta_{CO}\cdot\theta_{OH})$$

$$R = \frac{c_{HCHO}}{c_{HCHO2M}}$$

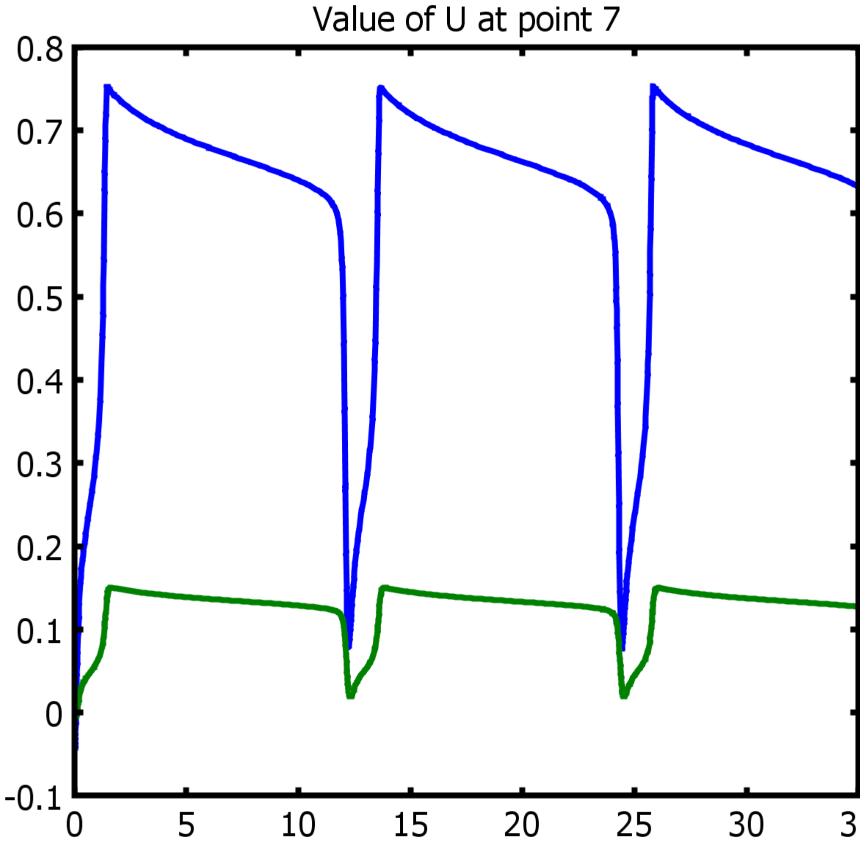
- Doyeon's model worked for 2M solution of HCHO
- This model also takes account concentration and applied constant current in range 10mA to 30mA

Electrochemical oscillations

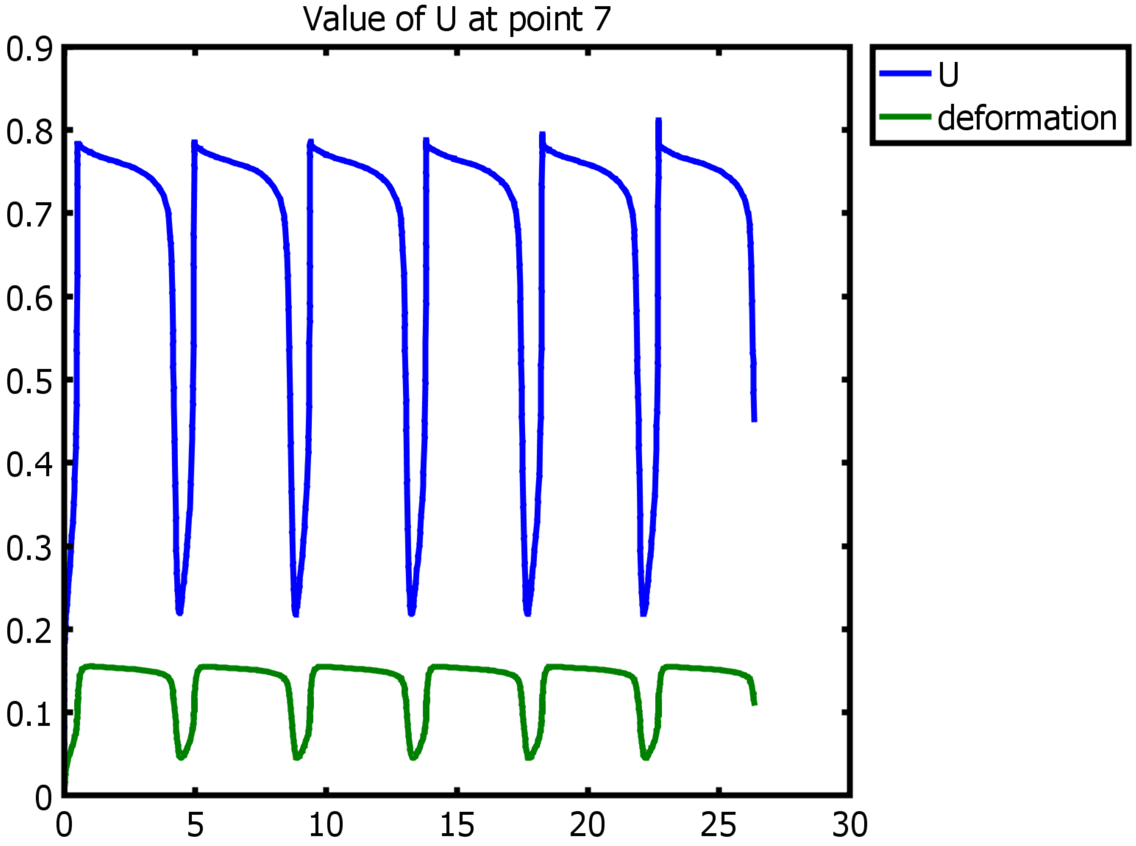


Displacement and voltage oscillations

1M HCHO, 25mA/cm2



3M HCHO, 25mA/cm2



Further goals

- Check all units and numbers. Specially everything related to diffusion layer.
- Better physical justification for addons to Doyeon's equations