Finite element simulations of the bending of the IPMC sheet

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ABSTRACT

Finite Element method is used to build and simulate an IPMC sheet. The physical bending of the realistic Nafion sheet due to the drift of counter-ions (e.g Na+) and dragged water in applied electric field are simulated. The effect of the concentration of counter-ions near the electrodes are tried to relate to the physical bending of the IPMC sheet. Mechanical properties of nafion polymer and platinum coating have taken account separately while modeling bending. All simulations are time dependent, thus transient model and need for few additional parameters is explained. Some additional effects like voltage drop at more distance points from contacts instead of constant electric field are discussed. Also some electrochemical reactions leading to self oscillations are explained and simulated.

Keywords: Electroactive polymers, EAP, Finite element method, Electrochemical-mechanical analysis, Actuator, Coupled problem, Self-oscillating systems

1. INTRODUCTION

EAP-based electromechanical actuators are valuable for use in a number of applications starting with miniature robotics up to military and space. These actuators have light weight, noiseless motion, simple mechanical construction; large controlled displacement and good damage tolerance along with an ability to perform different movements like bending and contractions makes possible to use them as artificial muscles. In this letter we consider simulation of ionic polymer-metal composite (IPMC) materials with finite element method (FEM).

IPMC materials are highly porous polymer materials such as Nafion, Fleminon, Teflon, filled with some kind of ionic conductive liquid. There are water based IPMCs which operate in aquatic environment and conduction is caused by ions such as Na+, K+ dissociated in water. Ionic liquid based IPMCs do not need wet environment for operating. The sheet of the ionic polymer is coated with thin metal layer, usually platinum or gold. In applied electric field the freely movable cations inside the polymer migrate towards an electrode, causing expansion of the material at the one end of the sheet and contraction at the other end, which leads to bending of the sheet.

For simulating actuation of an IPMC sheet we need to solve coupled problems due to the complex nature of IPMC actuation. It involves working in different domains such as mechanical, electrostatic and mass transfer. XXX and YYY have already simulated mass transfer and electrostatic effects. We have used similar approach for these problems. However, new approach is introduced for mechanical bending of IPMC strip. By coupling those domains together we get enough accurate finite element model for an IPMC muscle sheet. It allows us using the model as a base for solving more complex problems, thus we have also introduced simulation of electrochemical reactions.

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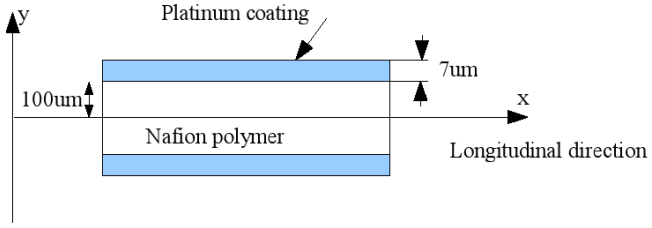

Figure 1. Illustration of domains and dimensions used in modeling.

1.1. Electrochemical oscillations

Spontaneous oscillations are common fenomenon in nature and it has been studied for many experiment, including electrochemical systems such as oxidation of organic materials and metals [REF]. Electrochemical systems exhibiting instabilities often behave like activator-inhibitor systems, where the potential of the electrode is an essential variable and takes on the role either of the activator or of the inhibitor. Under certain conditions the system can generate oscillations. We have conducted series of tests, where IPMC sheet have immersed into acidic formaldehyde, HCHO, solution and exposed to constant outer potential. However, measurements show current oscillations, which in turn result in oscillating bending of the IPMC sheet. Hence we have also introduced a model in this paper for describing such systems coupled with other physicals domains.

2. SIMULATION DETAILS

An IPMC sheet consists of backbone polymer and metal coating. We have used Nafion 117 coated with thin layer of platinum. Although, as it is written in the introduction that simulations in multiple physical domains are needed for getting bending model for an IPMC, most simulation is done in one mechanical domain - backbone polymer. Platinum coating is considered only in mechanics domain while calculating bending. So basically there are three mechanical domains as shown in Figure 1.

Most simulations are done for IPMC strip, 1.5cm long, 200um thick polymer coated with 7um thick platinum, for cantilever configuration - one end of the strip is not allowed to move. Gravitational forces are not considered in any following simulations.

2.1. Migration of cations

Nernst-Planck equations describes diffusion and convection and migration of charged particles under electric field. General form of the equation is

$$\frac{\partial C_i}{\partial t} + \nabla \cdot (-D_i \nabla C_i - z_i \mu_i F C_i \nabla \phi) = -\vec{u} \cdot \nabla C_i \tag{1}$$

where subscript i denotes species and C is concentration of species, μ is mobility of species, D is diffusion constant, T is absolute temperature, R is gas constant and ϕ is electric potential. This equations must be solved only for freely movable cations. As voltage is applied to the electrodes of the IPMC, all freely movable cations start migrating towards anode???, causing current in circuit. As ions cannot move beyond boundary of Nafion, charges start to accumulate, resulting in increase of electric field of opposite direction to applied one. So the electric field caused by charge distribution is described by Gauss' Law:

$$\nabla \vec{E} = \frac{F \cdot \rho}{\varepsilon} \tag{2}$$

where ρ is charge density, ε is absolute dielectric constant and E is the strength of the electric field and can be expressed also as $\nabla \phi = -E$. Steady state of the cations forms when electric field created by distribution

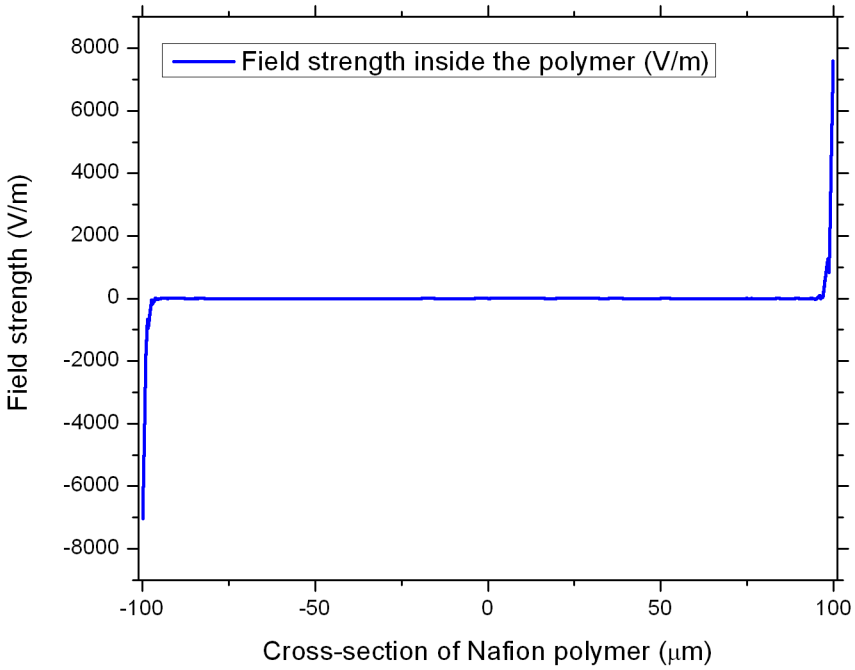

Figure 2. Electric field strength inside the IPMC in charge balance state. Notice that the field is zero inside the polymer, except really thin boundary layer.

of cations cancels out applied electric field, i.e. electric field strength inside the polymer is zero as shown in Figure 2. Charge distribution for Na+ ion concentration of $1200\frac{mol}{m^3}$ is shown in Figure 3. It is interesting to notice that there are differences in charge distribution only in really thin boundary layers.

2.2. Modeling actuation of an IPMC

Many authors have used Euler cantilever beam equation to model bending of an IPMC strip in cantilever configuration. [SOME ref's to authors?]. Though it describes position of the IPMC quite accurately for small displacements, it is not dynamical model - it does not show motion of the material in time. So using static Euler theory does not lead to really accurate time dependent model. Hence different approach is used for bending model: stiffness will be also considered when calculating. Importance of viscoelacity have been brought out also by some other authors like [REF].

2.2.1. Assumptions about bending mechanism

There are differences in charge distribution only in really thin boundary layers as we brought out before. General conclusion by many authors is that locally generated charge imbalance nearby platinum electrodes is main cause of bending of the IPMC [REFS]. We have defined longitudinal force in each point of the IPMC as follows:

$$\vec{F} = (A \cdot \rho + sgn(\rho) \cdot B \cdot \rho^2) \cdot \hat{x}, \tag{3}$$

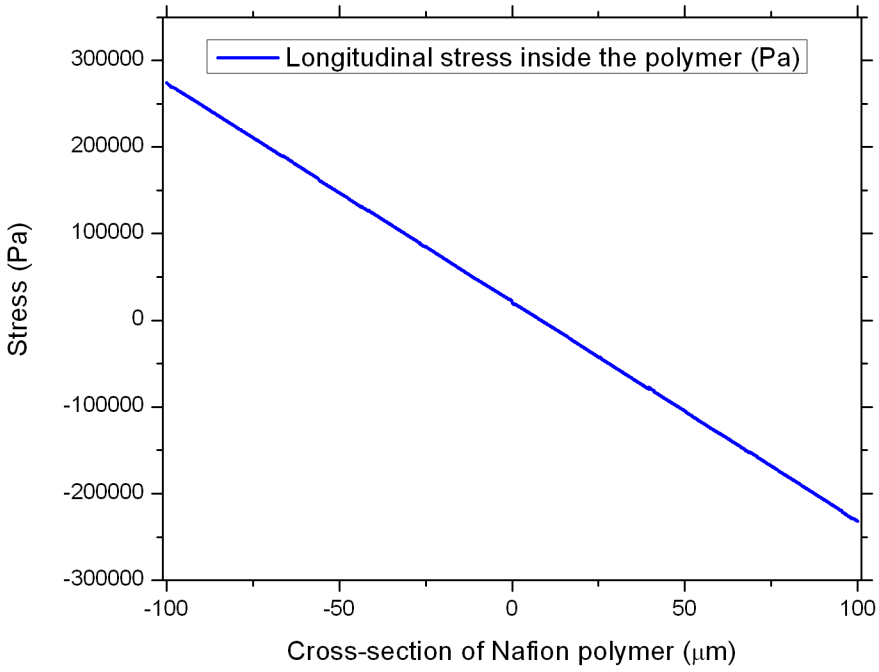

Figure 3. Cation distribution in charge balance state. Also longitudinal force according to modeling inside the polymer is shown. Notice that force grows faster near the boundaries of the polymer than cation distribution. The reason for that is quadratic term in force formula as shown in Equation 3. It is important to notice that the graph is somehow illustrative because real simulation maximum values for concentration and specially for stress are larger.

where ρ is charge density and A is a constant which could be found from different experiments. $sgn(\rho)$ is to preserve correct sign of excess charge. Basically the force is equivalent to the charge density and the shape of the force inside the polymer is also shown in Figure 3.

2.2.2. Math behind the bending

Finite element method for solving physical equations is very powerful and allows us to get more precise results than by using analytical methods. We used structural mechanics equations described in Comsol Multiphysics software package. Normal and shear strains are

$$\varepsilon_i = \frac{\partial u_i}{\partial x_i},\ \varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i}\right) \tag{4}$$

Where u denotes displacement, x denotes a coordinate and indeces i and j are from 1 to 3 and denote components correspondingly in x, y or z direction. As IPMC sheet in our simulations moves only in x-y plane, $\varepsilon_3 = 0$ and $\varepsilon_{23} = \varepsilon_{13} = 0$. Considering this we can write symmetric strain tensor in vector form and symmetric stress tensor in vector form as follows:

$$\varepsilon = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ 0 \\ 2\varepsilon_{12} \\ 0 \\ 0 \end{bmatrix},\ \sigma = \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \tau_{12} \\ \tau_{23} \\ \tau_{13} \end{bmatrix},\ \tau_{ij} = \tau_{ji}$$

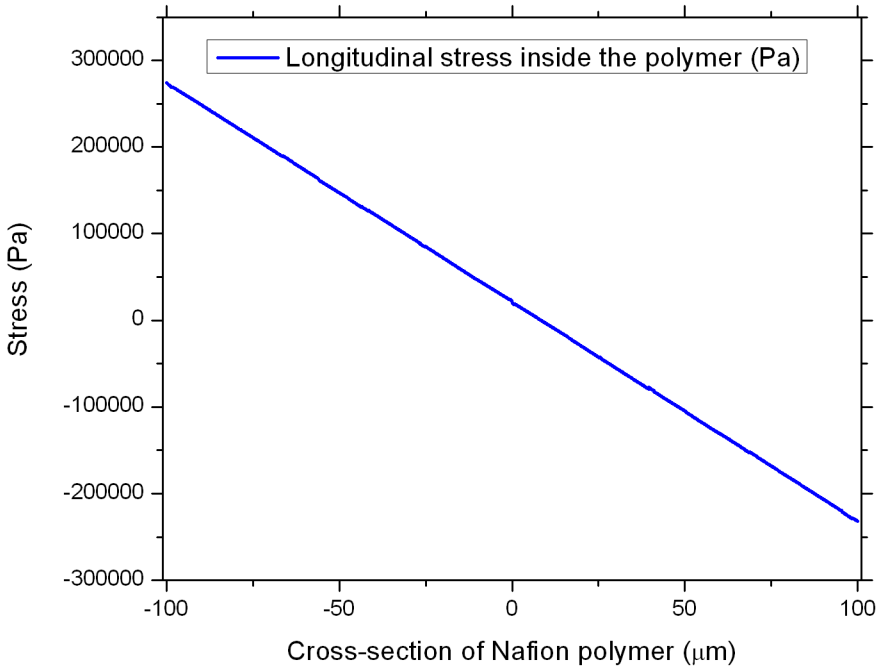

Figure 4. Longitudinal stress inside the polymer backbone in global coordinates.

and the stress-strain relationship is

$$\sigma = D\varepsilon. \tag{5}$$

D is elasticity matrix which is 6 x 6 matrix and consists of components of Young's modulus and Poisson's ratio. The system is in equilibrium if the following equation is satisfied:

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

which is basically Navier's equation for displacement. For instance, stress generated in the polymer is shown in Figure 4. The stress inside the platinum coating is very much bigger, thus it is not shown in the figure.

2.2.3. Transient analysis of bending

As our simulation is rather dynamic than static, we have to introduce equation for describing motion of the IPMC sheet. For that the Newton's Second law is used:

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

where second term in the equation is static Navier's equation. Dynamic part is introduced by the first term of the equation. This equation describes a system without damping.

Motion with Rayleigh damping model for system with single degree of freedom can be described

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

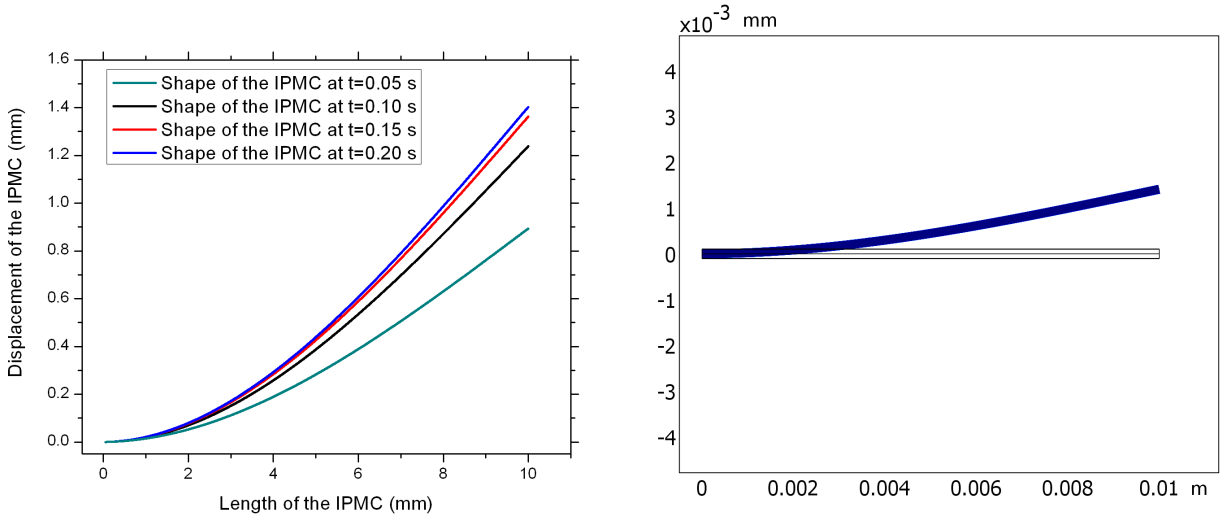

Figure 5. On the left: the shape of an IPMC muscle at different times (simulated with 2V, 1cm long strip). On the right: illustration of bending at t=0.2s

where ξ is damping parameter and can be expressed $\xi = \alpha m + \beta k$. Parameter m is mass and k is stiffness. Comsol Multiphysics uses similar form for systems with multiple degrees of freedom:

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

where c is constant used in static analysis.

All values used to simulate previously described equations are shown in Table 1.

Variable	Value	Dimension

Table 1. Values used in simulations.

2.3. Bending simulation results

Though there are couple of parameters in Equation 3, which depend on experimental results and are not very uniquely specified for all IPMC sheets, the simulates results predict the bending of an IPMC sheet precisely enough to use in further modeling problems. There are illustration of bending and the graph about the illustration shown in Figure 5. And as we are not modeling static problem, the time dependence of tip displacement of an IPMC muscle is shown in Figure 6.

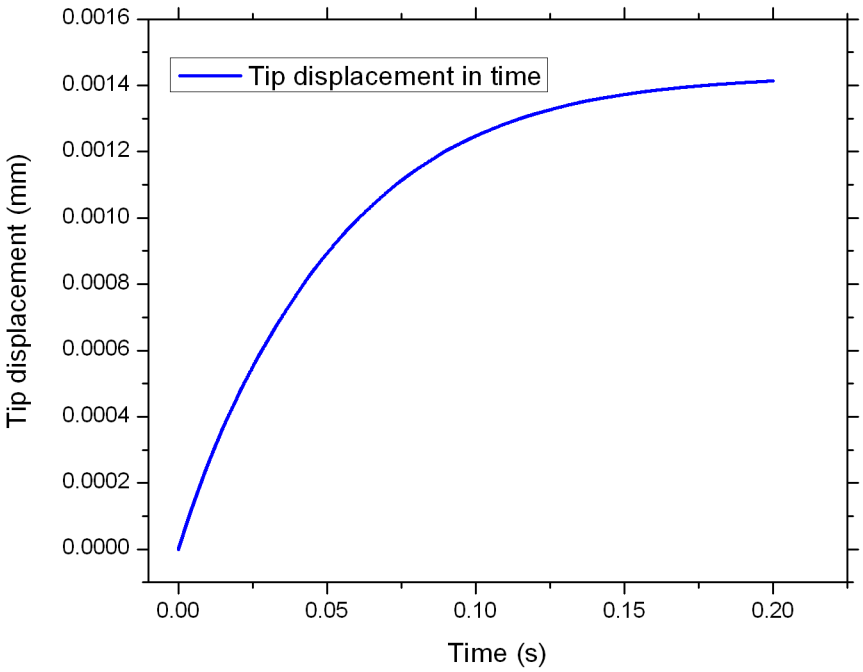

Figure 6. Tip displacement of an IPMC muscle in time.

By coupling previously described equations, we have developed good base model. Now it is possible to extend it by adding more equations to get physically meaningful results for more complicated problems. Next subsection of the article is good example, because electrochemical reactions which lead to self-oscillation of an IPMC muscle, are described and related to the model there.

2.4. Self-oscillations - coupling a problem of electrochemistry

We have conducted series of tests with IPMCs in formaldehyde (HCHO) solutions with constant applied electric field. Measurements show that current oscillations begin from potential of ca. 0.75V. Initial burst is caused by the reaction

$$CO_{ads} + OH_{ads} \rightarrow CO_2 + H^+ + e^- + 2*, \tag{6}$$

where ads denotes species adsorbed to the surface of platinum and * denotes an active platinum site. The result of this reaction is freeing up 2 sites which causes CO to adsorb again. These reactions lead to oscillating potentials which in turn lead to self-rhythmic motion of an IPMC.

Chronopotentiometry scans show that before reaction in Equation 6, following reactions occur:

$$HCHO + * \rightarrow Pt - CHO_{ads} + H^+ + e^- \tag{7}$$

$$Pt - CHO \rightarrow Pt - CO_{ads} + H^+ + e^- \tag{8}$$

$$H_2O + * \leftrightarrow Pt - OH_{ads} + H^+ + e^- \tag{9}$$

HCHO is dissociated on the electrode surface at lower anodic potential. Higher anodic potential causes dehydrogenation of water which results in water oxidation with intermediate (Pt-OH) formation.

2.4.1. Simulating electrochemical reactions

It is suggested by [REF] that concentration of HCHO near the platinum sufrace is important for reaction in Equation 7 and it is one factor for determing frequency of oscillations. We introduce double layer near the surface of one electrode in our simulation model.