An advanced finite element model of IPMC

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ABSTRACT

This paper presents an electro-mechanical Finite Element Model of an ionic polymer-Institute of Technology, Tartu University, Estoniametal composite (IPMC) material. Mobile counter ions inside the polymer are drifted by an applied electric field, causing mass imbalance inside the material. This is the main cause of the bending motion of this kind of materials. All foregoing physical effects have been considered as time dependent and modeled with FEM. Time dependent mechanics is modeled with continuum mechanics equations. The model also considers the fact that there is a surface of platinum and also a layer, where some amount of Pt is diffused into the polymer backbone. The described basic model has been under developement for a while and has been improved over the time. Simulation comparisons with experimental data have shown good harmony. Our previous paper described most of the basic model. Additionally, the model was coupled with equations, which described self-oscillatory behavior of the IPMC material. It included describing electrochemical processes with additional four differential equations. The Finite Element Method turned out to be very reasonable for coupling together and solving all equations as a single package. We were able to achieve reasonably precise model to describe this complicated phenomenon. Our most recent goal has been improving the basic model. Studies have shown that some electrical parameters of an IPMC, such as surface resistance and voltage drop are dependent on the curvature of the IPMC. The new model takes these effects into account to some extent. It has had an extra level of complexity to the model, because now all simulations are done in three dimensional domain. However, the result is advanced visual and numerical behavior of an IPMC with different surface characteristics.

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

1. INTRODUCTION

Electroactive polymer actuators have gained a lot of attention in many fields such as robotics and micro electronics. The advantages of EAP actuators are noiseless actuation, relatively simple mechanics and noiseless actuations. Additionally some EAPs, such as IPMCs, are able to function in aqueous environments. Those qualities make the materials possible to use as so called artificial muscles. In this paper we consider simulations of IPMC type material with the Finite Element Method. In this paper we consider three dimensional time dependent simulations of IPMC type materials with the Finite Element Method.

One of the most important qualities of IPMC materials is relatively large amplitude bending in response to electrical stimulations. An ion exchange polymer membrane, such as Nafion^{TM}, Teflon^{TM}, is covered with metal layers. The metal is typically platinum or gold. During the fabrication process the polymer membrane is saturated with certain solvent and ions. When voltage is applied to the metal electrodes, the ions start migrating due to the applied electric field. Migrating ions usually drag some solvent with them, causing expansion and contractions respectively near the surface layers. That in turn causes bending like actuation of IPMC sheet.

To simulate actuation of an IPMC sheet we need to solve coupled problems due to the complex nature of bending of an IPMC. Electrostatics, mass transfer and mechanical effects must be taken account to get a minimal functional base model which could predict actuation. Usually two dimensional time dependent model would be enough to get reasonable results. However, in this paper we consider three dimensional model of IPMC. This allows to take into account surface resistance changes for whole area of the metallic layer. Some authors have already simulated mass transfer and electrostatic effects. We used similar approach in our model. Toi has shown a Finite Element model including viscosity terms in transportation processes explicitly. The simulation is

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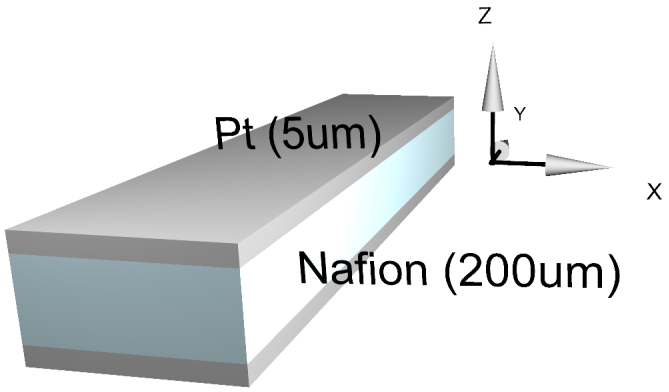

Figure 1. The IPMC strip, three-dimensional. The image is out of scale for illustrative purposes.

performed as time dependent and for three dimensions. However, the basis of the described model is a rectangular beam with 2 pairs of electrodes. Our approach for simulating mechanical bending is taking advantage of the numerical nature of FEM problems - we use continuum mechanics equations instead of analytical Euler beam theory which is more commonly used by authors. By coupling equations from different domains, we get a three dimensional simple model for an IPMC muscle sheet. That allows us to build up a more complex model. In the last section of this article the variable surface resistance model is discussed.

2. BENDING SIMULATIONS

We have used Nafion^{TM} 117, coated with thin layer of platinum in our experiments and therefore in theory. Mass transfer and electrostatic simulations are done only for backbone polymer. Continuum mechanics is taken into account for all domains, including the platinum coating. So there are two mechanical domains as shown in Figure 1.

All simulations are done for an IPMC strip of $200\mu m$ thick polymer coated with $7\mu m$ thick platinum, in a cantilever configuration - one end of the strip is fixed.

2.1. The base model

The cation migration in the polymer backbone is described by the Nersnt-Planck equation (Eq. (XXX)), which covers migration and diffusion part. The equation is:

$$\frac{\partial C}{\partial t} + \nabla \cdot (-D\nabla C - z\mu FC\nabla\phi) = -\vec{u} \cdot \nabla C, \tag{1}$$

where C is concentration, μ mobility of species, D diffusion constant, T absolute temperature, R universal gas constant, F Faraday constant, $\vec{u}$ velocity, z charge number and ϕ electric potential. The equations is solved only for cations as anions are fixed in the polymer backbone. As voltage is applied to the platinum electrodes, all free cations start migrating towards cathode, causing current in the outer electric circuit. As ions cannot move beyond the boundary of the polymer, local charge intensity starts to increase near the surface of the platinum electrodes, resulting in increase of electric field in the opposite direction to the applied one. This effect could be described by by Gauss' Law:

$$\nabla \cdot \vec{E} = -\Delta\phi = \frac{F \cdot \rho}{\varepsilon}, \tag{2}$$

where ρ is charge density, ε is absolute dielectric constant and E is the strength of the electric field and can be also expressed as $\nabla\phi = -\vec{E}$. The formed steady state of the cations is shown in Figure 2. The corresponding electric field distribution is also shown in Figure 2.

Many authors like Shahinpoor and Lee have used cantilever beam equation to model bending of an IPMC strip in cantilever configuration. Though using Euler beam model provides us analytical solution for a static

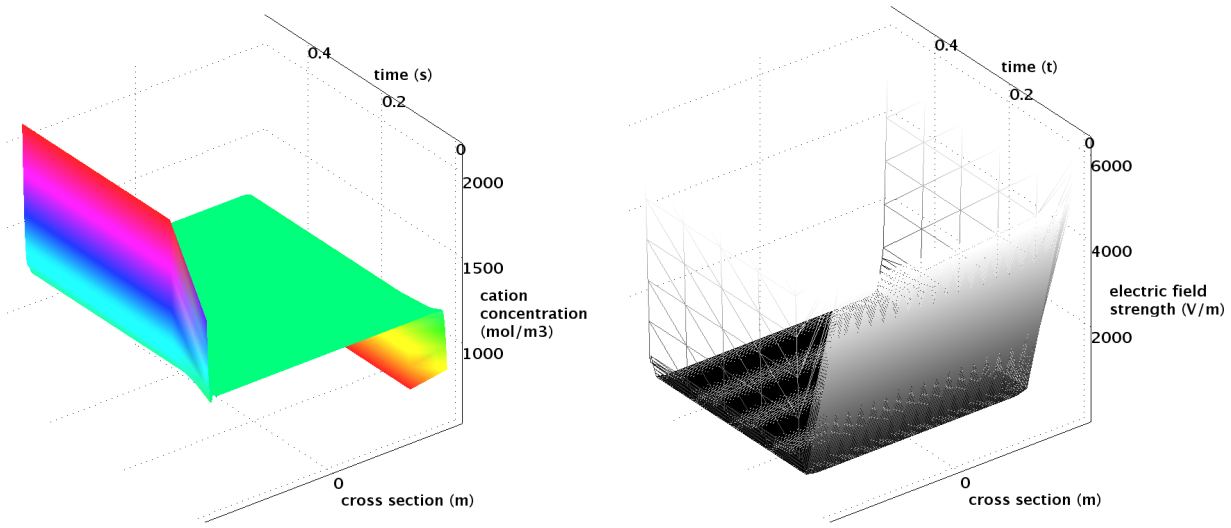

Figure 2. Cation concentration and electric field strength in an arbitrary cross section of an IPMC strip in time. The cross section length is 200 μm, and the time is from 0 to 0.5 s.

configuration, the model described in this paper is dynamic. So more accurate results could be obtained by using continuum mechanics model with damping. The tradeoff is slower calculation speed, but the given model is not intented for using in real time simulations anyway. Importance of viscoelasticity has been brought out also by some other authors like Richardson and Newbury.

There are differences in charge distribution only in really thin boundary layers as shown in Figure. As many authors have concluded, only the boundary layers cause the bending. The longitudinal force per unit cube in each point in the polymer of an IPMC is defined as follows:

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

where ρ is charge density and A and B are constants which could be fitted from different experiments.

To relate the force in Eq. 3 to the physical bending of an IPMC sheet, almost the same approach is used as in . Except this time all equations are solved in three dimensisons. These equations are described in Comsol Multiphysics structural mechanics software package. Normal and shear strain are defined as

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

where u is the displacement vector, x denotes a coordinate and indeces i and j are from 1 to 3 and denote components correspondingly to x, y, or z direction. The general stress-strain relationship is

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

where D is 6×6 elasticity matrix, consisting of components of Young's modulus and Poisson's ratio. The system is in equilibrium, if the relation

$$-\nabla \cdot \sigma = \vec{F}, \tag{6}$$

is satisfied. This is Navier's equation for displacement. The values of Young's modulus and Poisson's ratios, which are used in the simulations, are shown in Table **??**.

As we are dealing with time dependent simulations, we have to describe the dynamics of actuation rather than statics. Besides, we also want to consider damping. The damping effect could be caused by material itself

and by the environment in which the IPMC is working. Therefore we use Rayleigh damping model to empirically describe the effect:

$$m\frac{d^2u}{dt^2} + \xi\frac{du}{dt} + ku = f(t), \tag{7}$$

where the damping parameter ξ is expressed as $\xi = \alpha m + \beta k$. The parameter m is a mass, k is a stiffness and α and β are correspondingly damping coefficients. By coupling Eq. (7) with Newton's equation, we get the the equation, which is describes the dynamics of an IPMC strip:

$$\rho\frac{\partial^2\vec{u}}{\partial t^2} - \nabla\cdot\left[c\nabla\vec{u} + c\beta\nabla\frac{\partial\vec{u}}{\partial t}\right] + \alpha\rho\frac{\partial\vec{u}}{\partial t} = \vec{F}. \tag{8}$$

The origin of the equation is coverd in and also in Comsol Multiphysics manual.

So far we have described the base model, which is usable in both two dimensional and three dimensional modeling. The parameters for given equations Eq. (1) - Eq. (8) are given in 1.

Variable	Value	Dimension	Comment
D_{cation}	$2\cdot10^{-9}$	$\frac{m^2}{s}$	Diffusion coefficient of cations, e.g Na+.
ε	$3.8\cdot10^{-5}$	$\frac{F}{m}$	From capacitance measurment of an IPMC.
μ	$8\cdot10^{-13}$	$\frac{mol\cdot s}{kg}$	From Nernst-Einsten relation $\mu = \frac{D}{R\cdot T}$ where $T = 293K$, $R = 8.31\frac{J}{mol\cdot K}$.
Y_N	$50\cdot10^6$	Pa	Young modulus of Nafion^{TM}.
Y_{Pt}	$169\cdot10^9$	Pa	Young modulus of platinum.
ρ_N	2600	$\frac{kg}{m^3}$	Density of Nafion^{TM}.
ρ_{Pt}	21500	$\frac{kg}{m^3}$	Density of platinum.
A	$5\cdot10^5$	$\frac{N\cdot m}{C}$	A constant in Eq. (7).
B	$3\cdot10^4$	$\frac{N\cdot m^4}{C^2}$	A constant in Eq. (7).
α	1	$\frac{1}{s}$	Mass damping parameter.
β	0.5	s	Stiffness damping parameter.

Table 1. Base model simulation values.

2.2. Extended model

The model described in the previous section is good for both two dimensional and three dimensional modeling. However, solving the base model in 3D domain does not give us any kind of extra information. Instead it adds some complexity such as more complicated meshing and increased solving times. The real use of the third dimension comes, when the model takes into account also the surface resistance of the electrodes.

The surface resistance is an interesting characteristic of an IPMC strip. Besides of being different for different IPMC sheets, it tends to depend on the curvature of the IPMC strip. On the other hand, the surface resistance is the parameter which could be rather easily changed. For instance it is possible to make some areas of the muscle sheet less conductive. That's the place where 3 dimensional model could be useful.

The idea of the extended model is to put together part of the electrical model, such as and the model described in the previous section. It means that the cation transportation and continuum mechanics is coupled to the surface resistance and effects due to that.

2.3. Meshing in three dimensional domain

Meshing in three dimensional domain is not as straightforward as it is for 2 dimensions. There are couple of things which should be taken account. First of all, two dimensions of an IPMC sheet are relatively large (in range of centimeters) but the thickness is really small, far less than a millimeter. Besides, the thickness is not a solid piece as two layers of metal coating are considered as separate domains. Therefore the tetrahedral mesh really cannot be used over all the domains as the degrees of freedom for calculations would be unreasonably large. That's why the mapped meshing is technique is used. Instead of tetrahedral fine mesh, the rectangular mesh is greated. The

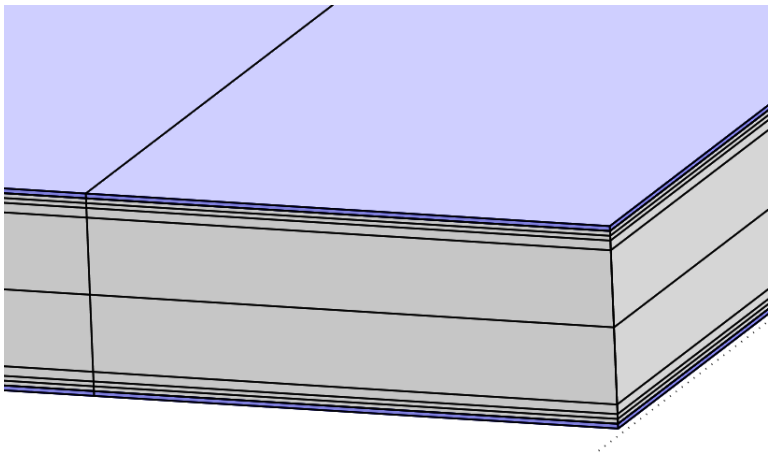

Figure 3. Meshing of an IPMC strip. One corner of the strip is shown. Notice the coarse mesh in the middle of the IPMC but fine mesh near the boundaries.

coarseness of the mesh is larger in the areas, where physical variables do not tend to change very rapidly. For instance the concentration of cations is rather smooth function in the middle of polymer backbone. Therefore areas around the surface layers contain finer mesh. As the problem is solved in number of physical domains, it is not really straightforward to determine the optimal mesh size analytically. Instead trial and error method could be used and after performing some simulations, the smoothness of the results could help to determine the optimal size of the mesh for future simulations. Example of a mesh could be seen in Figure 3.