MODELING ELECTRIC CURRENTS IN THE ELECTRODES OF IPMC

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ABSTRACT

This paper presents a Finite Element Analysis (FEA) of an ionic polymer-metal composite (IPMC) material. The IPMC materials are known to bend when electric field is applied on the electrodes and also produce a potential difference on the electrodes when bent. Several authors have used FEA to describe that fenomenon and therefore rather precise basic Finite Element (FE) models already exist. However, the focus of the current study is to model the electric currents in the electrodes. The basis of the calculations is the Ramo-Shockley theorem, which has been used in other areas of physics to describe the currents in a circuit due to a charge movement in a media. We have used the theorem to calculate the current density in the continuous electrodes of IPMC due to the ion migration in the backbone polymer. Along the current densities we are able to calculate exact voltage on the electrode at a given time moment. In this stage, the electrodes are modeled as static domains, i.e. no dynamic resistance changes have been considered. Although the work is still in progress, we have got some physically reasonable results to demonstrate and a section of the paper considers the extendibility of the model. Those results have already been previously published. However, in the paper we also consider some possible applications of the developed model and also couple of concerns in regard to modeling the whole IPMC in three dimensional domain with FE method.

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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 relatively simple mechanics and noiseless actuation. Additionally some EAPs, such as IPMCs [1], 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 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 stimulation. An ion exchange polymer membrane, such as Nafion, 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 predict the actuation, a good understanding of underlying processes must exist. 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 dimen-
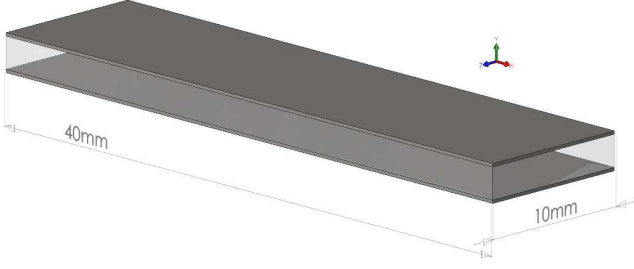
Figure 1. The simulated IPMC strip - the latter voltage drop simulation was conducted for an IPMC with the length of $40mm$. the image is out of scale for illustraion purpose.
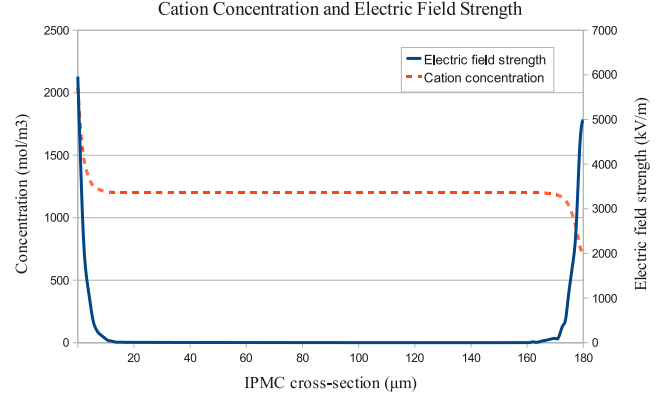

Figure 2. The cross section electric field and cation concentration in IPMC. the shape of the graphs is generally same for 2D and 3D simulations.

Table 1. The simulation input values for the base model.

Variable	Value	Dimension	Comment
D_{cation}	$2 \cdot 10^{-11}$	$\frac{m^2}{s}$	Diffusion const. [9]
ε	$2.5 \cdot 10^{-2}$	$\frac{F}{m}$	Measured.
μ	$8 \cdot 10^{-15}$	$\frac{mol \cdot s}{kg}$	$\mu = \frac{D}{R \cdot T}, T = 293K$

sional model of IPMC. This allows to take into account surface resistance changes for whole area of the metallic layer. Some authors [2–5] have already simulated mass transfer and electrostatic effects. We used similar approach in our model. Toi [6] has shown a Finite Element model including viscosity terms in transportation processes explicitly. The simulation is performed as time dependent and for three dimensions. However, the basis of the described model is a rectangular beam with 2 pairs of electrodes.

The current work is an extension of our already published paper [7], where we studied the surface currents and the voltage drops on the electrodes. The analytical surface resistance model is derived by Chen [8] for 2D domain.The proposed FE simulations work both in 2D and 3D domain. However, the current paper provides more insight of the challenges and some necessary optimizations in regard to the simulations.

2 THE SURFACE CURRENT MODEL

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. Surface current calculations are carried out for electrodes. All simulations are done for an IPMC strip of $180\mu m$ thick polymer coated with $3\mu m$ thick platinum, in a cantilever configuration - one end of the strip is fixed (see Figure 1).

2.1 The base model

The cation migration in the polymer backbone is described by the Nernst-Planck equation, which covers migration and diffusion part. The equation is:

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

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:

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

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 and corresponding electric field distribution is shown in Figure 2. The values of simulation constants are shown in Table 1.

So far we have described the base model, which is usable in both two dimensional and three dimensional modeling. Next we extend the model to include the current flow in the electrodes and also to estimate the currents and therefore the voltage distribution as well.
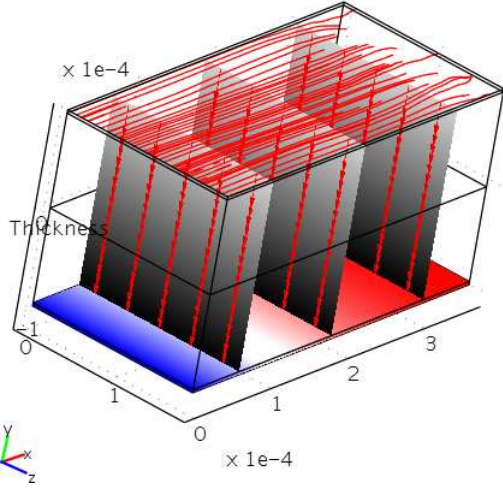
Figure 3. The base model with the surface electrode at $t = 0.1s$. The arrows indicate the cation flux and the whe white-gray area is the voltage inside the polymer. The blue-red area is the voltage on the electrode. Blue equals 0V.

2.2 Extended model

The model described in the previous section is sufficient for most cases and for two dimensional or three dimensional domains. However, solving the base model in three dimensional domain does not give us any kind of extra information - it is basically the same as an extended two dimensional solution. At the same time there is a significant increase in the complexity in terms of meshing and increase of degrees of freedom of the system, which in turns leads to longer solving times. The usefulness of the third dimension becomes eminent when the model takes into account also the surface resistance of the electrodes and when the surface resistance is not uniform in all three dimensions. The surface resistance is an important characteristic of an IPMC strip. Besides of being different for different IPMC sheets, it tends to depend on the curvature of the IPMC strip [10]. At the same time, the surface resistance is the parameter which could be rather easily altered. For instance, it is possible to make some areas of the muscle sheet less conductive. That is the case where three dimensional model would be more precise. However, even when the surface resistance is considered constant, there still exists a voltage drop along the surface and the extended model helps to take this into account.

The idea of the extended model is to put together part of the electrical model, which includes active resistances of the electrodes and the base model described in the previous section. Thus the cation transportation and continuum mechanics is coupled to the currents/voltages in the surface layers. Once having this model, the surface resistance could be easily varied as well, however, it is not in the scope of the current paper. The theory and simulation of electrical parameters of the electrodes are considered in the following subsections.
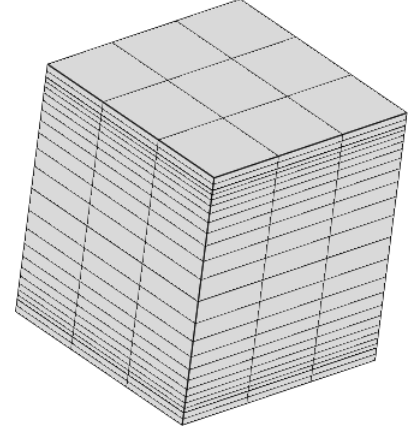

Figure 4. The mapped mesh generated with Comsol Multiphysics meshing tool.

2.2.1 Theory An IPMC strip with an external power source and connections form a closed electric circuit. There are roughly two types of conduction mechanisms in the circuit: electron conduction in the outer part of the circuit and the ion migration inside the IPMC. Even though the ions move only inside the polymer backbone, there is a connection between current in outer circuit and displacement of the ions. The theorem which is more often used in plasma physics [11], is called Ramo-Shockley theorem. It connects movement of charged particles in a confined space to the currents in a connected electric circuit. The theory, for instance, has been used to create a model of ion channels [12]. The equation to describe the current in the external circuit due to the relocation of the ions is:

$$I = \frac{1}{V} \sum_i q_i \times W(\vec{r}_i)_i \vec{v}_i, \qquad (3)$$

where j is the index of a particle, q is the charge, and v is the velocity of a particle. W corresponds to a electric field which would exist without any charged particles present [12]. By using Eq. (3), we can calculate the current flowing in an electrode. This in turn is related to the voltage in the surface layer. The surface layer could be depicted as a series of resistors which are also connected to the polymer. For this kind of two electrode system, the Eq. (3) could be written as

$$J = \frac{F}{d} \int_0^d \vec{f} \cdot \vec{dy}, \qquad (4)$$

where d is the distance between electrodes and $\vec{f}$ is the ion flux inside the polymer $\left[\frac{mol}{s\ m^2}\right]$, F is Faraday constant. The J is the current density in the electrode. By knowing the J, the current and also voltage in the electrode could be calculated using numerical methods. Therefore the electrodes are described as a

conductive media by using the following equation:

$$-\nabla \cdot \frac{\partial}{\partial t}\left(\varepsilon\nabla V\right) - \nabla \cdot \left(\sigma\nabla V\right) = 0, \qquad (5)$$

where V is voltage in the electrode, σ is electric conductivity. The boundary conditions of the electrodes are the applied voltage, the ground for the contact points, and insulation for all other surfaces.

2.2.2 Simulations

The Comsol Multiphysics Finite Element software package is used for simulations. That allowed to use predefined set of equations for different domains. The simulation of the metallic electrode coupled with the base model is rather complex, because the currents in the surface cause the changes of voltage acting on the polymer, i.e this is a feedback system. So building the model involved roughly the following steps:

1. A domain for base model was created and the equations (1) and (2) were applied - see Figure 3
2. Two surface layer domains were created. The surface layer characteristics were set close to the values of pure platinum. The conductivity, however, was altered a bit as the surface is not uniform for the case of IPMC. At the same time the conductivity was held constant during the simulation (see Figure 3). The electrode thickness was assumed to be around $3\mu m$. It is suggested though, that platinum layer is $1\mu m$, but as the model does not consider the platinum diffusion zone, the layer was chosen to be a bit thicker instead [13].
3. The voltage of the electrode boundaries which coincided with polymer, were set to be equal to the electric potential ϕ (see Eq. (2)).

Meshing in a three dimensional domain is not as straightforward as it is for two dimensions. There are couple of things which should be taken into account. First of all, two dimensions of an IPMC sheet are relatively large (width and length are in range of centimeters) but the thickness is really small, much less than a millimeter. In addition, the thickness consists of three layers - a polymer backbone and two layers of metal coating which are considered as separate domains. For this kind of system, the mapped mesh (as shown in Figure 4) would be the most reasonable. However, there are some restriction due to the solver (Comsol Multiphysics). The solver does not allow value projection for the mapped mesh. Therefore the tetrahedral mesh is used instead. The downside of that mesh is increased solution time.

The given model is able to calculate surface currents and voltages of the IPMC. Figure 5 the shows voltage drop along the surface quantitatively. As it could be seen, the voltage drop for ideal surface is rather negligible. This result is also supported by the rough measurements for some water based, platinum coated IPMCs produced in the lab. The small voltage drop for enhanced surface electrodes is also supported by Shahinpoor and Kim [14].
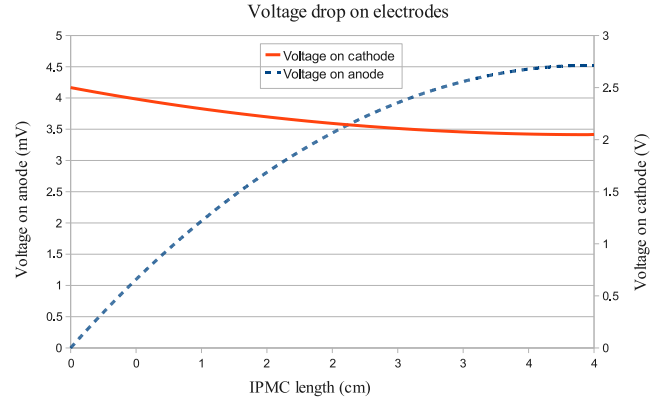

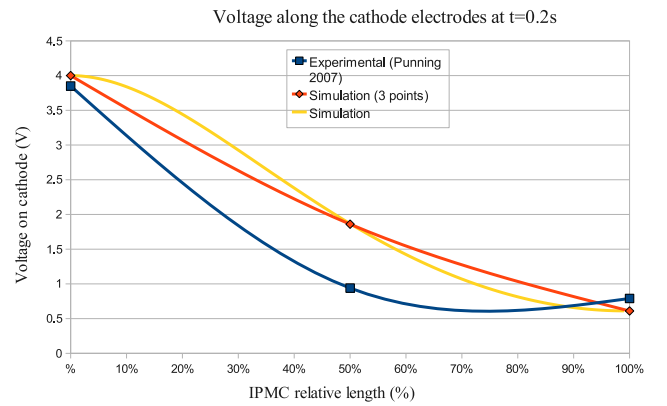Figure 5. The voltage drop on the electrodes at $t = 0.1s$.

Figure 6. The experimentla voltage drop at $(t = 0.2s)$. The simulated voltage drop and the experimental voltage drop show quite good correspondence specially at the ends of the sheet. However, in the middle of the sheet, the current example seems to be more non-linear than the simulation.

However, for some similar materials, rather large voltage drop at the beginning of actuation is observed [15, 16]. This could be caused by the bigger resistance or better ionic conductivity, which allows to draw more current near the electrode and therefore causing relatively bigger voltage drop along the electrode. To simulate the described situation, the surface resistance is altered in the model. The following relation was used for the cathode conductivity:

$$\sigma = \frac{\sigma_{Pt}}{10^5 \times x}, \qquad (6)$$

where x is the distance from the electrode and $\sigma_{Pt} = 8.9 \cdot 10^6\,S/m$. The value of x is kept always positive in the simulations and it should be noted that it stays considerably less than one. Figure 6 shows the simulated voltages and the voltages measured by Punning [16] at different points on the electrode. As the

voltage was measured only at three different locations on cathode, the experimental voltage curve could somewhat differ from the one interpolated on the graph.

3 DISCUSSION

The comparison of the developed model and experiments show that taking account the voltage drop in the electrode makes the model more precise. That could benefit even more when the developed continuum model is linked to a external circuit model to describe the system as one complete circuit. The developed model could be extended even further. As it is known, the platinum layer is not uniform on the surface of the polymer [1]. Therefore the resistance of the platinum is also somewhat increasing at the bottom layers, so by suggesting different resistance profiles, the model could be tuned to be more precise. Another benefit what could have when considering the surface electrodes, is the estimation the of heat generation on the electrodes.

3.1 Required optimizations

However, as it is brought out in the earlier sections of this paper, the model is rather complex and the calculations are time consuming. This limits the usage of the model. However, there are some things which could be done to optimize the model and therefore reduce the solution time.

For the three-dimensional model, the number of meshed elements is very large and therefore the solver must deal with more than a hunderd thousand degrees of freedom. As brought out before, the current solver does not allow using the mapped meshing due to the projection restrictions. So the goal is to generate as efficient tetrahedral mesh as possible. One way to achieve that is to test other preprocessors besides Comsol's integrated one. For instance, we have already tested Gmsh [17] meshing for a small piece of IPMC with electrodes (see Figure 7).

Another possible way to reduce the calculation time is to use a scaled model of IPMC - at least for the preliminary results. Final calculations could be done with a full scale model, however, the reduced scale helps significantly save the model development time. In some extent, we have used this for the current simulations already. To further simplify the calculations, timesteps could be used. It means that the static model is used for electrodes and by using a scripting language, we could solve the model for different timesteps. This would result close to the surface dynamic model.

Yet not explored area is using the weak form for the electrodes. As the coupling is complicated and nonlinear, the weak form (see Eq. (7)) could give us way better convergence. For the general equation

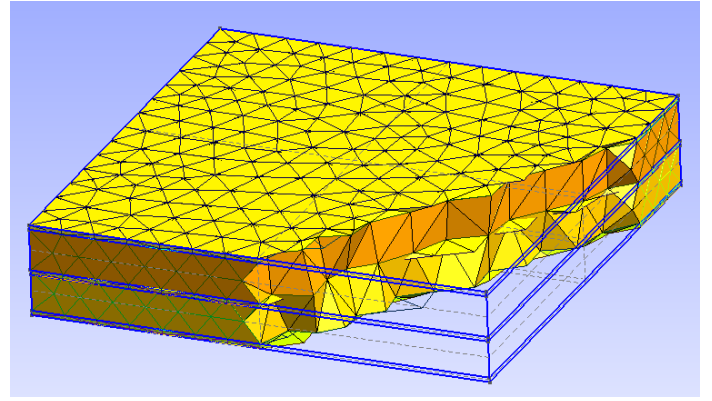$$\nabla \cdot \Gamma = F, \qquad (7)$$

Figure 7. A tetrahedral mesh for an IPMC with electrodes. Generated using Gmsh.

in the domain Ω, the weak form

$$\int_\Omega \nu \nabla \cdot \Gamma \, dA = \int_\Omega \nu F \, dA \qquad (8)$$

is obtained by multiplying the Eq (7) by a test function ν.

So as it could be seen, although the proposed model gives some physically reasonable results, it still requires more development. Though not suitable for real-time systems, the model could still be used in material development process to quantitatively validate the material properties. Furthermore, if only the purpose of a model is to describe bending of the IPMC in the linear region, then considering the voltage drop on the electrode would not contribute to the outcome significantly and could be omitted.

4 CONCLUSIONS

We have developed a base model to model the simple physical processes such as ion migration and electric field change in an IPMC. In this paper we have extended the base model to three dimensions, added surface electrodes and modeled the currents and voltage drop on them. Some improvements in meshing techniques have been necessary to be able to solve the three dimensional model within reasonable time, though even more improvements are necessary. To get the full use of the three dimensional model, the variable surface resistance part could be added later without significantly increasing the complexity of the existing model. The method used to calculate the currents in external circuit was derived from Ramo-Shockley theorem, mostly known in other fields of physics. Although the developed model gives physically meaningful results, more optimizations are needed to improve the model in terms of solution time and convergence. After the improvements, the model will be applicable for variety of IPMCs to estimate the current consumption and the voltage drop on the electrodes.

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