Dynamic Surface Resistance Model of IPMC

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ABSTRACT

Studies have shown that electrical parameters such as voltage drop and surface resistance are in correlation with curvature of IPMC. The electrical current in the surface of an IPMC could be calculated from the movement of the counter ions inside the polymer backbone of the IPMC. By using FEM we can calculate voltage drop in the platinum electrodes along the IPMC sheet. To get the relation between the voltage drop and current density, we use Ramo-Shockley theorem. The calculated voltage could again be applied as an input to the base model to calculate the curvature. This results in the Finite Element Model of an IPMC, which could be used for simulating basic actuation of an IPMC and furthermore, dynamic voltage changes on the electrodes. The current paper proposes a dynamical model of an IPMC with surface resistance taken into account. Also the voltage drop along the surface and overall currents are studied.

Keywords: Electroactive polymers, EAP, IPMC, Finite Element method, Actuator, Coupled problem, Surface resistance.

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 NafionTM, 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 dimensional 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. Toi⁶ 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.

In current work we do not explicitly calculate the bending of the material, rather the research puts emphasis on the study of surface currents and the voltage drops in the electrodes. The analytical surface resistance model is derived by Chen⁷ for 2D domain. The model proposed in the current paper considers simulations both in 2D and 3D domain. The base model is similar to the ones described above. However, the model for a metallic surface layer is introduced, i.e the electric currents and the voltage drop have been considered as well.

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Figure 1: The simulated IPMC strip - the latter voltage drop simulation were conducted for an IPMC with the length of 40mm. The image is out of scale for illustrative purposes.

2. THE DYNAMIC SURFACE CURRENT MODEL

We have used NafionTM 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. Surfa 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:

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

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 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.

Variable	Value	Dimension	Comment
D_{cation}	$2 \cdot 10^{-11}$	$\frac{m^2}{s}$	Diffusion coefficient of cations, ⁸ e.g Na ⁺ .
ε	$2.5 \cdot 10^{-2}$	$\frac{F}{m}$	From capacitance measurement of an IPMC.
μ	$8 \cdot 10^{-15}$	$\frac{mol \cdot s}{kg}$	From Nernst-Einstein relation $\mu = \frac{D}{R \cdot T}$ where $T = 293K$, $R = 8.31 \frac{J}{mol \cdot K}$.

Table 1: Simulation values of the base model.



Figure 2: Cross section electric field and cation concentration in IPMC. The shape of those graphs is generally same for 2D and 3D simulations. The profile of the graph is physically reasonable, however, the maximum values seem to be too high,⁹ so more work is needed to establish better boundary conditions.

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.

2.2.1. Theoretical background

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:

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

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

$$J = \frac{F}{d} \int_0^d \vec{f} \cdot d\vec{y},\tag{4}$$

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:

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

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. Extended model 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 4a
- 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 4b). 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. Therefore the tetrahedral mesh really cannot be used over all the domains as the degrees of freedom for calculations would be unreasonably large. That is why the mapped meshing technique is used. Instead of tetrahedral fine mesh, the rectangular coarser mesh is created. The coarseness of the mesh is larger in the areas, where values of the variables do not change very rapidly. For instance the concentration of cations is rather smooth function in the middle of polymer backbone. The problem of that kind of mesh is that not all integration techniques could be used. Example of a mesh could be seen in Figure 3.

The given model is able to calculate surface currents and voltages of the IPMC. The Figure 5 shows qualitatively how the voltages and currents could possibly distribute on the electrode surface at the beginning of



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.



(a) A base model without surface electrode. The arrows perpendicular to the surface denote the flux direction at the time t = 0.1. The surface slice color indicate the voltage drop.



(b) A base model with the surface electrode around t = 0.1s. The arrows indicate the cation flux and the white-gray area of the slices indicates the voltage inside the polymer. The blue-red area indicates the voltage on the grounded electrode - blue equals to 0.

Figure 4: Base model (a) and the model with electrodes (b). The initial model is scaled, so that the length of the IPMC is $400\mu m$ and the width is $200\mu m$.



Figure 5: The figure illustrates the simulated surface current densities at the time moment 0. The top layer is the metal electrode and the bottom "box" is the polymer. The red lines are streamlines of the current and the blue-yellow area represents isosurfaces of the same current density. The voltage is applied to the left boundary of the electrode.

actuation and Figure 6 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

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:

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

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 7 shows the simulated voltages and the voltages measured by Punning¹⁶ 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.

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. 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.



Figure 6: The voltage drop on the surfaces of the electrodes at t = 0.1s. Notice that the anode voltage drop is measured in millivolts rather than in volts.



Voltage along the cathode electrodes at t=0.2s

Figure 7: The experimental voltage drop at the beginning of the actuation phase (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.

Though the proposed model gives some physically reasonable results, it still requires more development. The results do not converge very well for larger time values and the way the coupling between the surface voltage and the voltage on the polymer boundary is done, could introduce a rather large error.

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. The developed model gives physically meaningful results and after some improvements could be applicable for variety of IPMCs to get estimates of current consumption and generated heat.

ACKNOWLEDGMENTS

The authors from University of Nevada, Reno (UNR) acknowledge the financial support from the U.S. National Science Foundation (Award#: 0713075). We also acknowledge the financial support from the European Science Foundation DoRa programme and CRDF-ETF joint grant no. ESE1-2902-TR-07.

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