Finite Element Modeling of Electrochemical-Poroelastic Behaviors of Conducting Polymer Films*

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Abstract
A computational modeling is established for the electrochemical-poroelastic behavior of conducting polymers (CPs) such as polypyrrole. The three-dimensional continuum modeling given by Della Santa et al. for the passive, poroelastic behavior of CPs is extended to the formulation for the active, electrochemical-poroelastic formulation according to Onsager-like laws, which is combined with the one-dimensional equation for ionic transportation. The validity of the finite element formulation for these governing equations has been illustrated by numerical studies for the passive and active responses of polypyrrole films.

Key words: Computational Mechanics, High Polymer Materials, Structural Analysis, Biomaterials, Electrochemistry, Poroelasticity, Finite Element Method, Stress Relaxation

1. Introduction

The following advantages are possessed by the actuators using conducting polymers such as polypyrrole: (i) generation of large forces (several ten times as large as human muscles), (ii) simple structures and light weight, (iii) noiseless, (iv) operation by low voltage (1~2 volts). The development, application and production of such actuators are expected in the fields of robotics, biomedical engineering and micro-electro-mechanical systems (1)-(5).

The deformation of expansion and contraction of a conducting polymer film in an electrolyte bath takes place, due to the coming in and out of electrolyte caused by the pressure difference between the inside and outside of the film. This is a passive, poroelastic behavior (1)-(3). When turning on electricity between a conducting polymer film and electrolyte, the deformation of expansion and contraction of the conducting polymer film is accelerated by the insertion and de-insertion of ions, which is an active, electrochemical-poroelastic behavior (1)-(3). The polypyrrole doped with relatively small anions such as ClO₄⁻ expand and contract due to the insertion and de-insertion of the anions (oxidation and reduction), which is classified as anion-driven actuators (4),(5). On the other hand, anions do not move in the polypyrrole doped with relatively large anions such as DBS (Dodecyl Benzene Sulfonate), which expands and contracts due to the insertion and de-insertion of cations (reduction and oxidation). It is classified as cation-driven actuators (4),(5).

Della Santa et al. (1)-(3) derived governing equations of continuum modeling based on poroelasticity theory for the response of conducting polymer actuators using polypyrrole. They compared one-dimensional theoretical solutions for the passive, poroelastic behavior...
with the experimental results, however, details of the formulation for the active, electrochemical-poroelastic behavior was not given. On the other hand, Tadokoro derived governing equations for the electrochemical-mechanical behaviors of ionic-conducting polymer-metal composites (IPMCs) such as Nafion membrane with platinum electrodes accompanied by the ionic movement under an electric field, the mechanism for expansion and contraction of which differs from that of conducting polymers such as polypyrrole. The finite element modeling for the electrochemical-mechanical behavior of ionic-conducting polymer-metal composites was given by Toi and Kang(7)(8).

The purpose of the present study is to establish computational modeling for the electrochemical-poroelastic behavior of conducting polymers to support design and development of the actuators using conducting polymers such as polypyrrole. The three-dimensional continuum modeling given by Della Santa et al.(1)(3) based on Biot’s poroelasticity theory(9) is extended to the formulation for the active, electrochemical-poroelastic behavior according to Onsager’s law(10), which is combined with the one-dimensional ionic transportation equation given by Tadokoro et al.(6) to construct the system of governing equations. The governing equations are discretized by the finite element method. Numerical calculations are conducted for the passive, poroelastic behavior and the active, electrochemical-poroelastic behavior, the results of which are respectively compared with the theoretical solution(1) and the experimental results(2) to illustrate the validity of the present modeling.

The finite element modeling for the electrochemical-poroelastic behavior of conducting polymer films and the computational results for polypyrrole films are described in section 2 and section 3, respectively. Section 4 contains concluding remarks.

2. Finite Element Formulation of Governing Equations for Electrochemical-Poroelastic Behaviors of Conducting Polymer Films

2.1 Stiffness Equations for Poroelastic Solids

According to Biot’s theory(9), the equilibrium equation of poroelastic solids containing fluid is given as follows:

\[
\frac{\partial \sigma^f_{ij}}{\partial x_j} = 0
\]  

(1)

where

\[
\sigma^f_{ij} = \sigma^s_{ij} + \sigma^f_{ij}
\]

(2a)

\[
\sigma^s_{ij} = \frac{E}{1 + \nu} \epsilon^s_{ij} + \frac{\nu E}{(1 + \nu)(1 - 2\nu)} \epsilon^s \delta_{ij}
\]

(2b)

\[
\sigma^f_{ij} = -\beta P \delta_{ij}
\]

(2c)

in which the following notations are used: \(\sigma^s_{ij}\), total stress; \(\sigma^f_{ij}\), stress in solid; \(\sigma^f_{ij}\), stress in fluid; \(x_j\), Cartesian coordinates; \(E\), Young’s modulus; \(\nu\), Poisson’s ratio; \(\epsilon^s_{ij}\), strain in solid; \(\epsilon^f\), volumetric strain in solid; \(\delta_{ij}\), Kronecker’s delta; \(\beta\), porosity; \(P\), pressure.

Neglecting external force components, the virtual work principle equivalent to Eq. (1) is expressed by the following equation:

\[
\int_V \delta \left( [\epsilon]_T + [\Delta \epsilon]_T \right) \left( [\sigma] + [\Delta \sigma] \right) dV = 0
\]

(3)

where \([\epsilon]_T\): total strain vector, \([\sigma]_T\): total stress vector, \(\delta\): variation, \(\Delta\): increment and \(V_e\): finite element region. Using Eq. (2a), Eq. (3) can be rewritten as
\[
\int_V \delta [\Delta \varepsilon]^{T} [\Delta \sigma'] dV = - \int_V \delta [\Delta \varepsilon]^{T} [\Delta \sigma^f] dV
\quad (4)
\]

The displacement increment \( \{\Delta u\} \) and the pressure increment \( \Delta P \) in each element are assumed as follows:
\[
\{\Delta u\} = [N_u] \{\Delta u_N\}
\quad (5a)
\]
\[
\Delta P = [N] \{\Delta P_N\}
\quad (5b)
\]

where \([N_u]\) and \([N]\) are the shape function matrices of eight-node hexahedron elements. \(\{\Delta u_N\}\) and \(\{\Delta P_N\}\) are the nodal displacement increment vector and the nodal pressure increment vector, respectively. Using Eqs. (2b) and (2c), the solid stress increment vector \(\{\Delta \sigma^s\}\) and the fluid stress increment vector \(\{\Delta \sigma^f\}\) are respectively expressed by the following equations:
\[
\{\Delta \sigma^s\} = [D^s] [\Delta \varepsilon] = [D^s] [B] [\Delta u^N]\quad (6a)
\]
\[
\{\Delta \sigma^f\} = -\beta [H]^T \Delta P
\quad (6b)
\]

where \([B]\): strain-nodal displacement matrix for solid, \([D^s]\): stress-strain matrix for solid and \([H]\): coefficient matrix determined by Eq. (2c).

Substituting Eqs. (6a) and (6b) into Eq. (4), the following three-dimensional element stiffness equation for poroelastic solids can be obtained:
\[
[K] \{\Delta u_N\} = \beta [B^s]^T \{\Delta P_N\}
\quad (7)
\]

Where
\[
[K] = \int_V \{B\}^T \{D^s\} \{B\} dV
\quad (8a)
\]
\[
[B^s] = \int_V \{B\}^T \{H\} \{N\} dV
\quad (8b)
\]

### 2.2 Poisson’s Equation for Pressure

According to Onsager’s law\(^{(10)}\), the relations among the ionic flux \(J\), the mass flux \(V^f\), the electric potential gradient \(\nabla \varphi\) and the pressure gradient \(\nabla P\) can be expressed as follows:
\[
J = K_{11} \nabla \varphi + K_{12} \nabla P
\quad (9a)
\]
\[
V^f = K_{21} \nabla \varphi + K_{22} \nabla P
\quad (9b)
\]

Calculating divergence of both hand sides of Eqs. (9a) and (9b) and eliminating \(\nabla^2 \varphi\), the following equation is used:
\[
\text{div } V^f = \frac{\partial \varepsilon^f}{\partial t}
\quad (10)
\]

Then, using the relation concerning the passive, poroelastic behavior\(^{(11)}\):
\[
\frac{\partial \varepsilon^f}{\partial t} = -\frac{(1 - \beta)}{f} \nabla^2 P
\quad (11)
\]

and Biot’s equation of continuity\(^{(9)}\):
\[
\frac{\partial \varepsilon^i}{\partial t} = -\frac{\beta}{1 - \beta} \frac{\partial \varepsilon^f}{\partial t}
\quad (12)
\]

the following Poisson’s equation for pressure in the case of electrochemical response can be
derived:
\[
\frac{\partial e^s}{\partial t} = C_1 \frac{-\beta}{(1-\beta)} \nabla J + C_2 \frac{\beta}{f} \nabla^2 P \tag{13}
\]

where \( f \) is a coefficient representing permeability of fluid in porous solids, which is called the frictional coefficient between solid and fluid\(^{(1)}\).

In each finite element, the volumetric strain rate of solid and the electric density rate are assumed as follows:

\[
\frac{\partial e^s}{\partial t} = \left[N_1\right] \dot{e}_N^s \tag{14a}
\]
\[
\nabla J = -\frac{\partial c}{\partial t} = -\left[N_1\right] \dot{e}_N^c \tag{14b}
\]

The basic equation for Galerkin finite element formulation of Eq. (13) is expressed by the following equation:

\[
\int_V \left\{ \left[N_1^T\right] \frac{\partial e^s}{\partial t} + C_1 \frac{\beta}{(1-\beta)} \nabla J - C_2 \frac{\beta}{f} \nabla^2 P \right\} dV = 0 \tag{15}
\]

Substituting Eqs. (14a) and (14b) into Eq. (15), the following equation can be obtained:

\[
\int_V \left\{ \left[N_1^T\right] \left[N_1\right] \dot{e}_N^s \right\} dV = -C_1 \frac{\beta}{(1-\beta)} \int_V \left\{ \left[N_1^T\right] \left[N_1\right] \dot{e}_N^c \right\}
\]
\[- C_2 \frac{\beta}{f} \int_V \left\{ \frac{\partial \left[N_1^T\right]}{\partial x} \frac{\partial \left[N_1\right]}{\partial x} + \frac{\partial \left[N_1^T\right]}{\partial y} \frac{\partial \left[N_1\right]}{\partial y} + \frac{\partial \left[N_1^T\right]}{\partial z} \frac{\partial \left[N_1\right]}{\partial z} \right\} dV \tag{16}
\]

From Eq. (16), the following equation for pressure can be obtained:

\[
\left[S_1\right] \dot{e}_N^c = C_1 \frac{\beta}{(1-\beta)} \left[S_1\right] \dot{e}_N^c - C_2 \frac{\beta}{f} \left[A_1\right] \left[P^c\right] \tag{17}
\]

### 2.3 Evolution Equation of Volumetric Strain Rate

Substituting Eq. (13) into the following relation which holds for the passive, poroelastic behavior:

\[
\frac{(1-\nu)E}{(1+\nu)(1-2\nu)} \nabla^2 e^s = \beta \nabla^2 P \tag{18}
\]

the following evolution equation of the volumetric strain for the electrochemical-poroelastic behavior can be obtained:

\[
L \nabla^2 e^s = \frac{1}{C_2} \frac{\partial e^s}{\partial t} + \frac{C_1}{C_2} \frac{\beta}{(1-\beta)} \nabla J \tag{19a}
\]

where

\[
L = \frac{(1-\nu)E}{f(1+\nu)(1-2\nu)} \tag{19b}
\]

The basic equation of Galerkin finite element formulation of Eq. (19a) is expressed by the following equation:

\[
\int_V \left\{ \left[N_1^T\right] \left(L \nabla^2 e^s - \frac{1}{C_2} \frac{\partial e^s}{\partial t} - \frac{C_1}{C_2} \frac{\beta}{(1-\beta)} \nabla J \right) \right\} dV = 0 \tag{20}
\]

Substituting Eqs. (14a) and (14b) into Eq. (20), the following equation can be obtained:
\[ \int_V [N]^T [N] \dot{\epsilon}_N^e \, dV = C_1 \frac{\beta}{1-\beta} \{ [N]^T [N] \dot{\epsilon}_N \} \]

\[ - C_2 J \int_V \left( \frac{\partial [N]^T}{\partial x} \frac{\partial [N]}{\partial x} + \frac{\partial [N]^T}{\partial y} \frac{\partial [N]}{\partial y} + \frac{\partial [N]^T}{\partial z} \frac{\partial [N]}{\partial z} \right)^\prime \{ \dot{e}_N \} \, dV \]

From Eq. (21), the following evolution equation of the volumetric strain can be obtained:

\[ [S] \dot{e}_N = C_1 \frac{\beta}{1-\beta} [S] \dot{\epsilon}_N - C_2 J[A] \dot{e}_N \] 

(22)

2.4 Ionic Transportation Equation

Turning on electricity of conducting polymer films in an electrolyte bath, the insertion and de-insertion of ions take place, which accelerates the deformation of expansion and contraction. Moving ions in the electrolyte bath are subjected to the forces due to viscous resistance, diffusion and electricity, the balance of which leads to the following differential equation with respect to the total electric charge \( Q(x,t) \) :

\[ \eta \frac{\partial Q(x,t)}{\partial t} = kT \frac{\partial^2 Q(x,t)}{\partial x^2} - \frac{\partial Q(x,t)}{\partial x} \times \left[ \frac{e}{\varepsilon_s S_x} \left[ \int_0^1 i(\tau) \, d\tau + Q(x,t) - Q(x,0) \right] \right] \]

(23)

Assuming that the electrodes in the polymer film and the electrolyte are located respectively at \( x = 0 \) and \( x = d \), the initial and boundary conditions are as follows:

\[ \{ Q(x,0) \} = N_v e S_x c_o x \]

(24a)

\[ \{ Q(0,t) \} = 0, \]

\[ \{ Q(d,t) \} = N_v e S_x c_o d \]

(24b)

where \( i \) is the electric current. The notations for the other symbols contained in Eqs. (23), (24a) and (24b) are given in Table 2. It should be noted that the ionic movement in the polymer film is assumed to be similar to that in the electrolyte bath for simplicity.

The electric charge density \( c(x,t) \) is calculated by the following equation, using the obtained total charge:

\[ Q(x,t) = N_v e S_x \int_0^x c(\xi,t) \, d\xi \]

(25)

Zero slope is assumed as the boundary conditions for the electric charge density.

The finite element formulation is conducted for Eqs. (23) and (25). The total electric charge \( Q(x,t) \) is linearly interpolated in each element:

\[ \{ Q(x,t) \} = [N] \{ Q_e \} = \left[ 1 - \frac{x}{h} \right] \frac{Q_e}{h} \]

(26)

where \( Q_e \) and \( Q_j \) are the total charge at nodes. \( h \) is the element length. The finite element formulation by Galerkin method is conducted for Eq. (23).

\[ \int_0^h [N]^T \left\{ \eta \frac{\partial Q(x,t)}{\partial t} - kT \frac{\partial^2 Q(x,t)}{\partial x^2} + \frac{\partial Q(x,t)}{\partial x} \times \left[ \frac{e}{\varepsilon_s S_x} \left[ \int_0^1 i(\tau) \, d\tau + Q(x,t) - Q(x,0) \right] \right] \right\} \, dx = 0 \]

(27)
Substituting Eqs. (26) and (27), the following ordinary differential equation system for the total charge can be obtained:

\[
\begin{bmatrix}
A_{11} & A_{12} \\
A_{21} & A_{22}
\end{bmatrix}\begin{bmatrix}
\dot{Q}_N \\
\dot{Q}_V
\end{bmatrix} + \begin{bmatrix}
B_{11} & B_{12} \\
B_{21} & B_{22}
\end{bmatrix}\begin{bmatrix}
Q_N \\
Q_V
\end{bmatrix} = 0
\]  

where

\[
\begin{bmatrix}
A_{11} & A_{12} \\
A_{21} & A_{22}
\end{bmatrix} = \begin{bmatrix}
\frac{h}{3} & h \\
\frac{h}{6} & h
\end{bmatrix}
\]  

(29a)

\[
\begin{bmatrix}
B_{11} & B_{12} \\
B_{21} & B_{22}
\end{bmatrix} = \begin{bmatrix}
kT - \frac{e}{2\eta_i \varepsilon_S S_x} \left[ \int_0^1 \text{d}(\tau(d\tau)) \right] + B_1 & -\frac{kT}{\eta_i h} + \frac{\Delta t e}{2\eta_i \varepsilon_S S_x} \left[ \int_0^1 \text{d}(\tau(d\tau)) \right] + B_2 \\
-kT & -\frac{e}{2\eta_i \varepsilon_S S_x} \left[ \int_0^1 \text{d}(\tau(d\tau)) \right] + B_3 & \frac{kT}{\eta_i h} + \frac{e}{2\eta_i \varepsilon_S S_x} \left[ \int_0^1 \text{d}(\tau(d\tau)) \right] + B_4
\end{bmatrix}
\]  

(29b)

\[
B_1 = -\frac{e}{\eta_i \varepsilon_S S_x} \left[ \frac{1}{3} (Q_j(x,t) - Q_j(x,0)) + \frac{1}{6} (Q_j(x,t) - Q_j(x,0)) \right]
\]

\[
B_3 = -\frac{e}{\eta_i \varepsilon_S S_x} \left[ \frac{1}{6} (Q_j(x,t) - Q_j(x,0)) + \frac{1}{3} (Q_j(x,t) - Q_j(x,0)) \right]
\]  

(29c)

Conducting the finite element formulation by Galerkin method for Eq. (25) relating the total charge with the charge density, the following equation can be obtained:

\[
\int_0^1 [N]^T \frac{\partial Q(x,t)}{\partial x} \left[ N_d e S_c(x,t) \right] dx = 0
\]  

(30)

Substituting Eq. (26) into Eq. (30), the following equation can be obtained:

\[
\begin{bmatrix}
C_{11} & C_{12} \\
C_{21} & C_{22}
\end{bmatrix}\begin{bmatrix}
\dot{Q}_N \\
\dot{Q}_V
\end{bmatrix} = \begin{bmatrix}
D_{11} & D_{12} \\
D_{21} & D_{22}
\end{bmatrix}\begin{bmatrix}
Q_N \\
Q_V
\end{bmatrix}
\]  

(31)

where

\[
\begin{bmatrix}
C_{11} & C_{12} \\
C_{21} & C_{22}
\end{bmatrix} = \begin{bmatrix}
\frac{N_d e S_x h}{3} & \frac{N_d e S_x h}{6} \\
\frac{N_d e S_x h}{6} & \frac{N_d e S_x h}{3}
\end{bmatrix}
\]  

(32a)

\[
\begin{bmatrix}
D_{11} & D_{12} \\
D_{21} & D_{22}
\end{bmatrix} = \begin{bmatrix}
-\frac{1}{2} & \frac{1}{2} \\
-\frac{1}{2} & \frac{1}{2}
\end{bmatrix}
\]  

(32b)

By summing up Eq. (28) for all elements and integrating with respect to time using a numerical integration scheme such as Euler method, time history of the total charge can be obtained. The charge density is calculated from Eq. (31).
2.5 Computational Procedure

Computational procedure for the active, electrochemical-poroelastic behavior using finite element equations given in the preceding subsections is as follows. The electric charge density is obtained from the global system forms of Eqs. (28) and (31). The volumetric strain rate is obtained from the global system form of Eq. (22) by using the electric charge density rate and the volumetric strain. The pressure is calculated from the global system form of Eq. (17) by using the volumetric strain rate and the electric charge density rate. The displacement increment is calculated from the global system form of Eq. (7) by using the pressure increment. The stress increments in solid and fluid are calculated from Eqs. (6a) and (6b) by using the displacement increment and the pressure increment. These procedures are repeated at each small time increment intervals until the final time.

3. Results of Finite Element Analysis

3.1 Analysis of Passive, Poroelastic Behaviors

The passive, poroelastic behavior of a polypyrrole film as shown in Fig. 1 has been simulated. Giving the polypyrrole film an initial strain in z-direction, the stress relaxation phenomenon due to the insertion of fluid has been analyzed by using the material parameters given in Table 1. When the initial pressure in the polypyrrole film is lower than in the surrounding electrolyte, the insertion of the electrolyte into the polypyrrole film takes place, which causes increase of the internal pressure, increase of the stress in solid and relaxation of the total stress with time. Figure 2 shows the finite element results for the time variation of the pressure distributions. In Fig. 3, the finite element results for the time histories of the internal pressure, the stress in solid and the total stress are compared with the theoretical solution given by Della Santa et al. (1). The validity of the present analytical algorithm is confirmed from these results.

Table 1  Material parameters for passive, poroelastic response analysis

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial strain</td>
<td>$e_0 = 0.00340909$</td>
</tr>
<tr>
<td>Poisson’s ratio</td>
<td>$v = 0.412$</td>
</tr>
<tr>
<td>Frictional coefficient</td>
<td>$f = 1.29 \times 10^{20} (Nsm^4)$</td>
</tr>
<tr>
<td>Young’s modulus</td>
<td>$E = 1290 (MPa)$</td>
</tr>
<tr>
<td>Porosity</td>
<td>$\beta = 0.108$</td>
</tr>
<tr>
<td>Time increment</td>
<td>$\Delta t = 0.005 sec$</td>
</tr>
</tbody>
</table>
3.2 Analysis of Electrochemical-Poroelastic Behaviors

The natural stress relaxation phenomenon under no electric current was analyzed in the preceding subsection. In the present subsection, supposing cation-driven actuators, the active, electrochemical-poroelastic behavior is analyzed. The dimensions of a polypyrrole film are the same as in Fig. 1. Table 2 shows the material parameters used in the analysis.
Figure 4 shows the calculated results in which the pressure rise is accelerated by the insertion of cations into the film, taking the polypyrrole film side as negative and the electrolyte side as positive. Figure 4(a) shows the assumed three types of electric current patterns whose durations of stepwise currents are two seconds (case 1), four seconds (case 2) and six seconds (case 3), respectively. Figure 4(b) shows time variations of the electric charge density distribution in the film \(0 \leq x \leq 0.0175\) and the electrolyte bath \(0.0175 < x \leq 0.175\), from which it can be seen that the charge density rises with time by the insertion of cations into the film. Figure 4(c) is the time-history of the pressure in the film. Comparing with the passive behaviors analyzed in the preceding subsection, the pressure rises faster when turning on the electricity and it gradually approaches the pressure of electrolyte by the passive de-insertion of electrolyte after turning off the electricity. These results can be considered to be reasonable.

Figure 5 shows the calculated results in which the pressure rise is decelerated by the de-insertion of cations into the film, taking the polypyrrole film side as positive and the electrolyte side as negative. Figure 5(a), 5(b) and 5(c) show the electric current patterns, the time variation of the electric charge density distribution (case 3) and the time-history of the pressure in the film. The pressure decreases by the de-insertion of cations when turning on the electricity and it gradually approaches the pressure of electrolyte by the passive insertion of electrolyte after turning off the electricity, which can also be considered to be a reasonable result.

Another analysis has been conducted for the elongation and contraction behavior of a polypyrrole film (length: 90mm, width: 1mm, thickness: 32 \(\mu\)m) subjected to a stepwise positive and negative current cycle (amplitude: 5mA, frequency: 62.5sec). Figure 6 shows the calculated time history of the length which agrees well with the experimental result(2). As most of the physical constants for the polypyrrole film are unknown, they have been assumed so as to give the calculated result in good correspondence with the experimental result, based on those for Nafion membranes(7),(8) as shown in Table 2.

Table 2: Material parameters for active, electrochemical-poroelastic response analysis

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coefficient of viscosity for hydrated Na(^+) moving through membrane</td>
<td>(\eta_1 = 1.18 \times 10^{11} \text{ (N} \cdot \text{s/m}^2))</td>
</tr>
<tr>
<td>Boltzmann constant</td>
<td>(k = 1.380 \times 10^{-23} \text{ (N} \cdot \text{m} / \text{K}))</td>
</tr>
<tr>
<td>Absolute temperature</td>
<td>(T = 293\text{ (K)})</td>
</tr>
<tr>
<td>Elemental charge</td>
<td>(e = 1.6 \times 10^{-19} \text{ (C)})</td>
</tr>
<tr>
<td>Dielectric constant of hydrated Nafion membrane</td>
<td>(\varepsilon_r = 2.8 \times 10^{-1} \text{ (C}^2 / \text{N} \cdot \text{m}^2))</td>
</tr>
<tr>
<td>Time interval</td>
<td>(\Delta t = 5 \times 10^{-4} \text{ s})</td>
</tr>
<tr>
<td>Space interval</td>
<td>(h = 2\mu\text{m})</td>
</tr>
<tr>
<td>Cross section area</td>
<td>(A_r = 34.2 \times 10^{-6} \text{ (m}^2))</td>
</tr>
<tr>
<td>Avogadro number</td>
<td>(N_a = 6.02 \times 10^{23} / \text{mol})</td>
</tr>
</tbody>
</table>
Fig. 4  Electrochemical-mechanical response of polypyrrole film (cation entering)

(a) current patterns  
(b) time variations of charge density distribution (case 3)  
(c) time histories of pressure

Fig. 5  Electrochemical-mechanical response of polypyrrole film (cation emitting)

(a) current patterns  
(b) time variations of charge density distribution (case 3)  
(c) time histories of pressure
From the above-mentioned numerical studies, the present computational modeling can be considered to be qualitatively reasonable, however, quantitative validation based on experiments remains as a future subject.

4. Conclusion

A computational modeling for the electrochemical-poroelastic behavior has been proposed to support design and development of actuators using conducting polymers such as polypyrrole. The three-dimensional continuum modeling given by Della Santa et al. based on Biot’s poroelasticity theory has been extended to the formulation for the active, electrochemical-poroelastic behavior according to Onsagar-like law, which is combined with the one-dimensional ionic transportation equation to construct the system of governing equations. Discretizing these equations by the finite element method, numerical studies have been carried out for the passive, poroelastic behavior and the active, electrochemical-poroelastic behavior of polypyrrole films. The former result and the latter result have been compared with the theoretical solution and the experimental result, respectively. The validity has been verified from a qualitative point of view. Lots of processes including determination of physical constants are necessary for quantitative validation, which are future subjects with the applications to the other conducting polymers such as polyaniline and the multi-dimensional modeling of ionic transportation equation.

References

(3) Della Santa, A. et al., Characterization and Modeling of a Conducting Polymer Muscle-Like Linear Actuator, Smart Materials and Structures, 6, (1997), pp.23-34.

