Mixed finite element modelling of cartilaginous tissues

by

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Abstract

Swelling and shrinking of cartilaginous tissues is modelled by a four-component mixture theory. This theory results in a set of coupled non-linear partial differential equations for the electro-chemical potentials and the displacement. For the sake of local mass conservation these equations are discretised in space by a mixed finite element method. Integration in time by backward Euler leads to a non-linear system of algebraic equations. A subtle solution strategy for this system is proposed and tested for one-dimensional situations.

Keywords: cartilaginous tissues, electro-chemical potentials, mixed finite elements, Darcy, Fick, Hooke.
Symbols

\( c \)  molar concentration of the fluid phase  \([\text{mol m}^{-3}]\)
\( c^\beta \)  molar concentration of ion \( \beta \) per unit fluid volume  \([\text{mol m}^{-3}]\)
\( c^{fc} \)  molar concentration of fixed charge per unit fluid volume  \([\text{mol m}^{-3}]\)
\( D^\beta \)  diffusivity of ion \( \beta \)  [-]
\( f^\beta \)  activity coefficient of ion \( \beta \)
\( F \)  Faraday's constant  \([\text{C mol}^{-1}]\)
\( K \)  hydraulic permeability  \([\text{m}^4 \text{N}^{-1} \text{s}^{-1}]\)
\( p \)  pressure of the fluid phase  \([\text{N m}^{-2}]\)
\( q \)  specific discharge  \([\text{m s}^{-1}]\)
\( q^\beta \)  flux of ion \( \beta \)  \([\text{mol m}^{-2} \text{s}^{-1}]\)
\( R \)  universal gas constant  \([\text{J mol}^{-1} \text{K}^{-1}]\)
\( t \)  time  \([\text{s}]\)
\( T \)  absolute temperature  \([\text{K}]\)
\( u \)  displacement  \([\text{m}]\)
\( v^\alpha \)  velocity of the \( \alpha \)-phase  \([\text{m s}^{-1}]\)
\( z^\beta \)  valence of ion \( \beta \)  [-]
\( z^{fc} \)  valence of fixed charge  [-]
\( \delta \)  dilatation  [-]
\( \epsilon \)  strain tensor
\( \lambda^\alpha \)  Lamé stress constant  \([\text{N m}^{-2}]\)
\( \mu \)  electro-chemical potential of the fluid phase  \([\text{N m}^{-2}]\)
\( \mu^\beta \)  electro-chemical potential of ion \( \beta \)  \([\text{J mol}^{-1}]\)
\( \mu^\alpha \)  Lamé stress constant  \([\text{N m}^{-2}]\)
\( \xi \)  voltage  \([\text{V}]\)
\( \rho^\alpha \)  apparent density of the \( \alpha \)-phase  \([\text{kg m}^{-3}]\)
\( \rho^\alpha \)  true density of the \( \alpha \)-phase  \([\text{kg m}^{-3}]\)
\( \sigma \)  stress tensor
\( \phi \)  porosity  [-]
\( \phi^\alpha \)  volume fraction of the \( \alpha \)-phase  [-]
\( \Phi^\beta \)  osmotic coefficient of ion \( \beta \)  [-]
1 Introduction

Cartilaginous tissues are soft hydrated tissues with strong swelling properties. They play an important role in joint lubrication and damping of dynamic forces in the human body. Their multi-component, non-homogeneous anisotropic nature complicates the mechanical analysis. Therefore experimental work on simplified geometric conditions should be combined with advanced finite element computations. The swelling and shrinking behaviour of cartilaginous tissues is caused by the flow of water that is bound to the charged solid skeleton of the porous tissue. The driving mechanism is an interplay of mechanical, chemical and electrical forces. Swelling and shrinking can be modelled by a four-component mixture theory [11, 7, 6] in which the deformable and charged porous medium is saturated with a fluid with dissolved cations and anions. The four-component mixture theory is based on balance equations for the solid matrix, the fluid, the cations and anions. The fluxes of the fluid and ions depend on the gradients of the electro-chemical potentials [14] of the fluid and the ions. The electro-chemical potentials are functions of the fluid pressure, the ion concentrations and the voltage. Furthermore, electro-neutrality must hold, which leads to an algebraic constraint. The solid matrix and fluid are assumed to be intrinsically incompressible and therefore a non-zero fluid flux divergence gives rise to swelling or shrinking of the porous medium. Alternatively, a gradient in the fluid pressure, ion concentrations or voltage results in flow of the fluid and ions [6]. The system of partial differential equations is discretised in space by a finite element method [4, 3] and integrated in time by a backward difference formula like backward Euler. Since there are several unknowns, a mixed finite element method [2, 15, 12] is used. A suitable choice for the approximation of the fluxes leads to a locally conservative scheme. This scheme results in a non-linear system of equations that needs to be solved iteratively. A subtle procedure is proposed and tested for a typical one-dimensional configuration.

2 Governing equations

The mixture theory is a continuum model that assumes that the different phases exist simultaneously at each point in space. Here two phases are considered, a fluid with dissolved mono-valent ions and a solid with attached ionic groups, respectively denoted by the indices $f$ and $s$. The true density of the $\alpha$-phase, where $\alpha = f, s$, is denoted by $\rho^\alpha = dm^\alpha/dV^\alpha$, where $dm^\alpha$ is the mass of the $\alpha$-phase in a small elementary volume $dV^\alpha$ containing only this phase. The porous medium is assumed to be initially homogeneous. Both the fluid and the solid phase are considered to be intrinsically incompressible. Moreover, it is assumed that the concentrations of dissolved ions and attached ionic groups are small. The assumptions imply that $\rho^f$ can be stated to be constant and uniform for both phases. Compression of the medium arises only because of a redistribution of the fluid and solid phases. The apparent density of the $\alpha$-phase in the mixture is defined as $\rho^\alpha = dm^\alpha/dV$, where
$dV$ is a representative elementary volume [1] of the medium. Let the volume fraction of the $\alpha$-phase be defined as $\phi^\alpha = dV^\alpha/dV$, then $\rho^\alpha = \phi^\alpha \rho^s$. For a binary porous medium $\phi = \phi^f$ is the porosity and thus $\phi^s = 1 - \phi$. Since the medium is assumed to be initially homogeneous, $\phi$ is initially uniform.

Conservation of mass for each phase implies

$$\frac{\partial \phi^\alpha}{\partial t} + \nabla \cdot (\phi^\alpha \mathbf{v}^\alpha) = 0, \quad \alpha = f, s,$$

where it is assumed that no sources or sinks exist. Here $\mathbf{v}^\alpha$ is the average velocity [1] of the $\alpha$-phase. Addition of these two equations gives

$$\nabla \cdot (\mathbf{q} + \mathbf{v}^s) = 0, \quad (1)$$

where the specific discharge relative to the solid matrix is defined as

$$\mathbf{q} = \phi (\mathbf{v}^f - \mathbf{v}^s).$$

No body forces such as gravity are assumed and the inertial terms are neglected. It is assumed that the solid matrix is entirely elastic and initially isotropic. The deformations are considered to be small enough such that the infinitesimal elastic assumption is valid. The shear stress associated with mixture deformation is assumed to be negligible in fluids. With these assumptions [13],

$$\nabla \cdot \mathbf{\sigma} = 0 \quad (2)$$

is obtained, where the stress tensor is defined by

$$\mathbf{\sigma} = (\lambda^s \delta - \rho) \mathbf{I} + 2\mu^s \mathbf{\varepsilon}. \quad (3)$$

In this formula $\rho$ is the fluid pressure, $\lambda^s$ and $\mu^s$ are the Lamé stress constants and $\mathbf{I}$ is the identity tensor. The dilatation is given by

$$\delta = \nabla \cdot \mathbf{u}, \quad (4)$$

and the strain tensor by

$$\mathbf{\varepsilon} = \frac{1}{2} \left( \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right), \quad (5)$$

where $\mathbf{u}$ is the displacement vector of the solid matrix. From the infinitesimal elastic assumption it follows that the boundary conditions are applied at the original position of the material. Now, (1) can be rewritten into the storage equation

$$\frac{\partial \delta}{\partial t} + \nabla \cdot \mathbf{q} = 0. \quad (6)$$
The variation of the porosity can be calculated by noting that conservation of mass for the solid phase can be written as
\[ \frac{\partial \phi}{\partial t} = (1 - \phi) \frac{\partial \delta}{\partial t}. \]

The infinitesimal elastic assumption implies that the term \( \mathbf{v}^s \cdot \nabla \phi \) can indeed be neglected [16]. It follows that
\[ \phi = 1 - (1 - \phi_0) e^{-\delta}, \] (7)

where \( \phi_0 \) is the initial porosity. Note that (7) can be replaced by \( \phi = \phi_0 + \delta \). However, it appears that (7) is more stable within the computational approach of the next section.

Conservation of mass for the dissolved ions implies
\[ \frac{\partial (\phi c^\beta)}{\partial t} + \nabla \cdot (\phi c^\beta \mathbf{v}^\beta) = 0, \beta = +, -, \]

where \( c^\beta \) is the molar concentration of ion \( \beta \) per unit fluid volume and \( \mathbf{v}^\beta \) is the average velocity of ion \( \beta \). The definition of the specific discharge implies that this equation can be rewritten as
\[ \phi \frac{\partial c^\beta}{\partial t} + c^\beta \frac{\partial \delta}{\partial t} + \nabla \cdot \mathbf{q}^\beta + \nabla \cdot \left( (c^\beta \mathbf{q}) \right) = 0, \beta = +, -, \] (8)

where the molar flux \( \mathbf{q}^\beta \) relative to the fluid is defined as
\[ \mathbf{q}^\beta = \phi c^\beta (\mathbf{v}^\beta - \mathbf{v}^f). \]

In deriving (8) the variation of the porosity is expressed in terms of the variation of the dilatation. Electroneutrality implies
\[ z^+ c^+ + z^- c^- + c^{fc} c^{fc} = 0, \]

where \( z^\beta \) is the valence of the dissolved ion \( \beta \). For a mono-valent salt, \( z^+ = +1 \) and \( z^- = -1 \). The superscript \( fc \) stands for fixed charge, i.e. the attached ionic groups, thus \( c^{fc} \) denotes the molar concentration of the attached ions per unit fluid volume. Conservation of fixed charge implies
\[ \frac{\partial (\phi c^{fc})}{\partial t} + \nabla \cdot (\phi c^{fc} \mathbf{v}^s) = 0. \]

From this equation it follows that
\[ \phi \frac{\partial c^{fc}}{\partial t} + c^{fc} \frac{\partial \delta}{\partial t} = 0, \]

and therefore
\[ c^{fc} = c_0^{fc} e^{-\delta/\phi_0}, \] (9)
where $c_{0}^{f_{c}}$ is the initial fixed charge concentration. Note that (9) can be replaced by 
$\phi = \phi_{0}c_{0}^{f_{c}}/\phi$. However, it appears that (9) is more stable within the computational approach of the next section.

In order to complete the system of equations, constitutive equations for the specific discharge and the molar flux are needed. For the specific discharge an extended Darcy’s law

$$q = -K \left( \nabla \mu + c^{+} \nabla \mu^{+} + c^{-} \nabla \mu^{-} \right) \tag{10}$$

is stated, where $K$ is the constant and uniform hydraulic permeability, and the electrochemical potentials $\mu$ are defined by

$$\mu = p - RT \left( \Phi^{+} c^{+} + \Phi^{-} c^{-} \right),$$
$$\mu^{\beta} = z^{\beta} F \xi + RT \ln \frac{f^{\beta} e^{\beta}}{c}, \quad \beta = +, -, \tag{11}$$

Here $R$ is the universal gas constant, $T$ is the absolute temperature, $F$ is Faraday’s constant, $\xi$ is the voltage and $c$ is the molar concentration of the fluid phase, which is assumed to be constant and uniform. The activity coefficient is defined by

$$f^{\beta} = \left( \frac{c^{\beta}}{c} \right)^{\phi^{\beta} - 1}, \tag{12}$$

where the osmotic coefficient $\Phi^{\beta}, \ 0 < \Phi^{\beta} \leq 1$, is constant and uniform. The definitions of the electro-chemical potentials and electro-neutrality imply that

$$q = -K \left( \nabla p - z^{f_{c}} c^{f_{c}} F \nabla \xi \right).$$

For the ion fluxes Fick’s laws

$$q^{\beta} = -\frac{D^{\beta}}{RT} \phi c^{\beta} \nabla \mu^{\beta}, \quad \beta = +, -, \tag{12}$$

are stated, where $D^{\beta}$ is the diffusivity. It follows that

$$q^{\beta} = -D^{\beta} \phi \left( \Phi^{\beta} c^{\beta} + \frac{F}{RT} z^{\beta} c^{\beta} \nabla \xi \right), \quad \beta = +, -. \tag{12}$$

Darcy’s law and Fick’s laws can be stated in terms of the electro-chemical potentials $\mu$ and $\mu^{\beta}$, or in terms of the variables $p$, $c^{\beta}$ and $\xi$. From physical considerations $\mu$ and $\mu^{\beta}$ are continuous, even if $c^{f_{c}}$ is not. Therefore we choose the electro-chemical potentials to be the primitive variables. From the definitions of the electro-chemical potentials and electro-neutrality it follows that

$$c^{\beta} = -\frac{1}{2z^{f_{c}}} z^{f_{c}} c^{f_{c}} + \frac{1}{2} \sqrt{\left(z^{f_{c}} c^{f_{c}}\right)^{2} + \frac{4c^{2}}{f^{+} f^{-}} \exp \frac{\mu^{+} + \mu^{-}}{RT}}, \quad \beta = +, -, \tag{13}$$

$$p = \mu + RT \left( \Phi^{+} c^{+} + \Phi^{-} c^{-} \right), \tag{14}$$

$$\xi = \frac{1}{z^{\beta} F} \left( \mu^{\beta} - RT \ln \frac{f^{\beta} e^{\beta}}{c} \right), \quad \beta = +, -. \tag{13}$$
The ion concentrations $c^\beta$ are clearly positive. Note that the activity coefficients $f^\beta$ depend on the ion concentrations by (11). For numerical stability it is preferable to use the expression for the voltage with $\beta = -$ if $z^{fc}$ is positive and vice versa.

The combination of the deformation of the porous medium and the flow of the fluid and ions results into a set of coupled equations (2–14) for the primitive variables $\mu$, $\mu^\beta$ and $u$. As boundary conditions we need suitable combinations of essential conditions for these variables or natural conditions for the normal components of $q$, $q^\beta$ and $\sigma$.

Consider the case that the porous medium is in contact with an electro-neutral bathing solution, i.e. the pressure $p_{out}$, the voltage $\xi_{out}$ and the ion concentrations $c^\beta_{out}$ are given. The bathing solution contains no fixed charges, so $c^\beta_{out} = c^\beta_{out} = c^\beta_{out}$. Since the electro-chemical potentials are continuous at the boundary,

$$
c^\beta = -\frac{1}{2z^\beta z^{fc} c^{fc}} + \frac{1}{2} \sqrt{(z^{fc} c^{fc})^2 + \frac{c^+_{out} c^-_{out} 4c^2_{out}}{z^+ f^- f^+}} \beta = +, -, $$

$$
p = p_{out} + RT \left(\Phi^+ c^+ + \Phi^- c^- - (\Phi^+_{out} + \Phi^-_{out}) c_{out}\right), $$

$$
\xi = \xi_{out} + \frac{RT}{z^\beta F} \ln \frac{f^\beta_{out} c^\beta_{out}}{f^\beta c^\beta}, \beta = +, -.
$$

In this specific situation $p$ is the osmotic pressure [14] and $\xi$ is the Nernst potential [10, 9]. The equation for $c^\beta$ is known as the Donnan equilibrium [11].

### 3 Finite element approximation

The set (2–14) consists of coupled non-linear equations. In order to deal with complicated geometries a finite element method is preferable. Standard finite elements [4, 3] result in continuous, piecewise polynomial approximations for the electro-chemical potentials $\mu$ and $\mu^\beta$. The specific discharge $q$ and the ion fluxes $q^\beta$ can then be obtained by numerical differentiation. The resulting vector fields are not conserving mass locally. In order to obtain locally conservative vector fields we choose to use mixed finite elements [2, 15, 12]. Assume that the $d$-dimensional domain $\Omega$ with boundary $\Gamma$ is polygonal. A regular triangulation [4] can be constructed by subdividing $\Omega$ into a collection $S_h$ of mutually disjoint subdomains $S \in S_h$, such that every subdomain is an interval ($d = 1$), a triangle or a rectangle ($d = 2$), or a tetrahedron or a brick ($d = 3$). The index $h$ measures the size of the largest subdomain. The primitive variables $\mu$ and $\mu^\beta$, and thus also $c^\beta$, $p$ and $\xi$, are approximated by piecewise constant functions. Since we want to derive a locally conservative scheme, the specific discharge $q$ and the ion fluxes $q^\beta$ are approximated by functions of Raviart-Thomas type of the lowest order [2, 15, 12]. The normal components of these functions are constant and continuous across inter-element boundaries. The displacement $u$ is approximated by a continuous, piecewise linear, bilinear (in case of rectangles) or trilinear (in case of bricks), vectorial function [4, 3]. Therefore the dilatation $\delta$, and thus the porosity $\phi$, are piecewise constant.

Using Green’s formula, the finite element approximation of (2–14) can be stated as follows.
Find $q$, $q^\beta$, $\mu$, $\mu^\beta$ and $u$ such that $q$, $q^\beta$ and $u$ fulfill suitable essential boundary conditions, and

\[
\begin{aligned}
\frac{1}{K} \int_\Omega q \cdot \bar{q} \, dx - \int_\Omega \mu \nabla \cdot \bar{q} \, dx - \int_\Omega \mu^+ \nabla \cdot (c^+ \bar{q}) \, dx - \int_\Omega \mu^- \nabla \cdot (c^- \bar{q}) \, dx \\
= - \int_\Gamma \mu n \cdot \bar{q} \, ds - \int_\Gamma \mu^+ n \cdot (c^+ \bar{q}) \, ds - \int_\Gamma \mu^- n \cdot (c^- \bar{q}) \, ds,
\end{aligned}
\]

\[
\frac{RT}{D^\beta} \int_\Omega \frac{q^\beta \cdot \bar{q}^\beta}{\phi c^\beta} \, dx - \int_\Omega \mu^\beta \nabla \cdot \bar{q}^\beta \, dx = - \int_\Gamma \mu^\beta n \cdot \bar{q}^\beta \, ds, \quad \beta = +, -, \]

\[
- \int_\Omega \nabla \cdot \bar{q} \tilde{\mu} \, dx - \int_\Omega \frac{\partial \delta}{\partial t} \tilde{\mu} \, dx = 0,
\]

\[
- \int_\Omega \nabla \cdot q^\beta \tilde{\mu}^\beta \, dx - \int_\Omega \nabla \cdot (c^\beta q) \tilde{\mu}^\beta \, dx - \int_\Omega \phi c^\beta \frac{\partial \delta}{\partial t} \tilde{\mu}^\beta \, dx
\]

\[
= \int_\Omega \frac{\partial c^\beta}{\partial t} \tilde{\mu}^\beta \, dx, \quad \beta = +, -, \]

\[
- \int_\Omega \mu \delta \, dx + \int_\Omega (\lambda^s \delta \bar{\delta} + 2\mu^s \varepsilon : \bar{\varepsilon}) \, dx
\]

\[
= RT \int_\Omega \left( \Phi^c c^+ + \Phi^c c^- \right) \delta \, dx + \int_\Gamma n \cdot \sigma \cdot \tilde{u} \, ds,
\]

for all test functions $\bar{q}$, $\bar{q}^\beta$, $\tilde{\mu}$, $\tilde{\mu}^\beta$ and $\tilde{u}$. Here $n$ denotes the outward normal at $\Gamma$. The test functions are of the same type as the search functions $q$, $q^\beta$, $\mu$, $\mu^\beta$ and $u$. However, if $q$, $q^\beta$ and $u$ fulfill some essential boundary conditions, then $\bar{q}$, $\bar{q}^\beta$ and $\tilde{u}$ fulfill the corresponding homogeneous boundary conditions.

Many combinations of boundary conditions are possible. We consider three choices:

- The porous medium slips along a no-flow boundary, i.e. $n \cdot q = 0$, $n \cdot q^\beta = 0$ and $n \cdot u = 0$, and all boundary integrals in (15) vanish.

- A normal force is applied to a no-slip and no-flow boundary, i.e. $n \cdot q = 0$, $n \cdot q^\beta = 0$ and $t \cdot u = 0$, where $t$ denotes any tangential vector at $\Gamma$. All boundary integrals in (15) vanish except the last one in which $n \cdot \sigma$ is given.

- The porous medium is in contact with an electro-neutral bathing solution through a rigid boundary, i.e. $u = 0$, and $\mu$ and $\mu^\beta$ are given in the boundary integrals in (15).

Integration of (15) by a suitable backward difference formula, e.g. backward Euler, leads to a non-linear system of equations. Note that the ion concentrations $c^\beta$ are given functions of the electro-chemical potentials $\mu^\beta$ as stated in (13). However, the activity coefficients $f^\beta$ depend on the concentrations $c^\beta$ by (11). The porosity $\phi$ depends on the displacement $u$ by (7) and (4).

Note that $\nabla \cdot (c^\beta \bar{q})$ in (15) is not well defined because $c^\beta$ is piecewise constant. Let some basis function $\bar{q}$ correspond to an inter-element boundary, then $c^\beta$ is defined as the harmonically weighed mean value of $c^\beta$ in the two neighbouring subdomains and $\nabla \cdot (c^\beta \bar{q})$ is used in the third and fourth integral in (15).
Consider the non-linear system of equations resulting from backward Euler. The assumption that \( c^\beta \) and \( \phi \) are known transforms the system into a linear one. It seems reasonable to assume that the porosity \( \phi \) changes gradually and can be taken at the old time level of a time step. Also the fixed charge concentration \( c^{fc} \) changes gradually by (9). So, the difference \( c^+ - c^- \) changes gradually by electro-neutrality, but the sum \( c^\pm = c^+ + c^- \) can change quickly. Now, \( c^\beta \) can be computed from \( \mu^+ \) and \( \mu^- \) by (13) if the activity coefficients are known. Since for \( \phi \) the value at the old time level is taken, the solution \( \mu^\beta \) of the linear system for fixed \( c^\beta \) can be denoted symbolically by \( \mu^\pm = A^{-1}(c^\pm) \ b (c^\pm) \), where \( A \) and \( b \) represent the matrix and right-hand side of the linear system. Now \( c^\pm \) can be computed by (13), i.e. \( c^\pm = f (\mu^\pm, c^\pm) \), where the dependence of \( f \) on \( c^\pm \) is generated by \( f^\beta \). Ergo, we obtain the non-linear system

\[
c^\pm = f (A^{-1}(c^\pm) \ b (c^\pm), c^\pm) .
\]  

This system can be solved by some iterative procedure for non-linear systems. In each iteration a linear system has to be solved. It should be observed that different scales are apparent in (15) that will result in a poorly scaled matrix in the linear system. Therefore the matrix \( A \) is replaced by the scaled matrix \( DAD \), where the diagonal matrix \( D \) is defined by

\[
D^2 = \text{diag} \left( \frac{L}{K}, \frac{LRT}{D^+\phi_0 c_f}, \frac{LRT}{D^-\phi_0 c_f}, \frac{K}{L}, \frac{D^+\phi_0}{LRT}, \frac{D^-\phi_0}{LRT}, \frac{\lambda^2 + 2\mu^\pm}{L} \right).
\]

Here \( L \) is a representative length scale.

### 4 Numerical simulations

We consider an uniaxial confined swelling and compression experiment (see figure 1) performed on a cylindrical sample of cartilage substitute. This sample, with a diameter of 4 mm and a height of approximately 1 mm, was made of out of a hydrogel with a similar material behaviour as cartilaginous tissue [6]. During experiments it degenerates less than cartilaginous tissue and it can be produced repeatedly with equal material properties.

The sample was put in an insulating confining ring. A piston on the top of the sample was loaded mechanically. A bathing solution flowed through a porous glass filter at the bottom of the sample. A change of the salt concentration of this solution generates a change in the boundary ion concentrations and pressure due to (13) and (14). In this confined swelling and compression device, the deformation of the sample and the voltage difference over the sample were measured [8].

During the experiment, the mechanical and chemical load were varied. Inspired by it, two numerical simulations are considered. Because of the essentially one-dimensional nature of the experiments, the numerical computations were performed for one-dimensional situations. All computations were done in MATLAB, where the non-linear system (16) was solved by the script fminsearch.
For both computations the length of the sample is $L = 10^{-3}$ m and the simulation time is $T = 3600$ s. Furthermore, $c = 55.4 \cdot 10^3$ mol m$^{-3}$, $c_{\text{in}} = 301$ mol m$^{-3}$, $D^+ = 4.4 \cdot 10^{-10}$ m$^2$ s$^{-1}$, $D^- = 6.7 \cdot 10^{-10}$ m$^2$ s$^{-1}$, $F = 96485.3$ C mol$^{-1}$, $\lambda^s + 2\mu^s = 0.2 \cdot 10^6$ N m$^{-2}$, $K = 5.5 \cdot 10^{-16}$ m$^4$ N$^{-1}$ s$^{-1}$, $R = 8.3145$ J mol$^{-1}$ K$^{-1}$, $T = 293$ K, $z^c = -1$, $\phi_0 = 0.945$, $\Phi^+ = \Phi^- = 1$.

As boundary conditions an inward force is applied to the left no-flow boundary, and at the right rigid boundary the porous medium is in contact with an electro-neutral bathing solution. As the initial condition $\sigma = -78 \cdot 10^3$ N m$^{-2}$ and $u = 0$ m are chosen. Therefore $\rho = 78 \cdot 10^3$ N m$^{-2}$. Let the ion concentration of the exterior fluid be given by $c_{\text{out}} = 150$ mol m$^{-3}$ with $\xi = 0$ V, then

$$\mu^+ = \mu^- = RT \log \frac{c_{\text{out}}}{c}. \quad (17)$$

Now the ion concentrations $c^\beta$ are given by (13) and $\mu = p - RT(c^+ + c^-)$.

For the first experiment $\sigma = 195 \cdot 10^3$ N m$^{-2}$ at the left boundary. All unknowns change immediately at $t = 0$ s, and finally another equilibrium will establish. At the final equilibrium the electro-chemical potentials $\mu$ and $\mu^\beta$ have the same value as for the initial state. However $\sigma$ and $p$ have changed, since the porous medium is compressed.

For the computations the interval is divided into 10 elements of length $h = 0.1$ mm and the time interval is chosen to be $\Delta t = 300$ s. The results are displayed in figure 2. For the second experiment the same initial conditions are chosen except $c_{\text{out}} = 450$ mol m$^{-3}$ with $\xi = 0$ V. The initial electro-chemical potentials $\mu^\beta$ follow from (17), the ion concentrations $c^\beta$ follow from (13) and $\mu = p - RT(c^+ + c^-)$. At $t = 0$ s the ion concentration of the exterior fluid changes to $c_{\text{out}} = 150$ mol m$^{-3}$ and therefore $\mu^\beta$ changes according
Figure 2: Numerical results for the first experiment: specific discharge $q$, cation flux $q^+$, anion flux $q^-$, displacement $u$, fixed charge concentration $c_f^c$, pressure $p$. 
to (17). Note that the ion concentrations $c^\theta$ at the right boundary cannot be determined directly since $c^{lc}$ is not known a priori. Let the initial value of $\mu$ be denoted by $\mu_0$ and its boundary value by $\mu_{bnd}$, then $\mu_{bnd} = \mu_0 - 2RT\Delta c_{out}$, where $\Delta c_{out} = 300$ mol m$^{-3}$. Again, all unknowns change immediately at $t = 0$ s and then evolve to equilibrium values. For the computations the same space and time discretisation as for the first experiment are chosen. The results are displayed in figure 3.

Note that the displacements are rather large. This implies that the infinitesimal elastic assumption is not fulfilled for the parameters at hand. However, we expect that the computational model will perform well for smaller strains. For large strains the assumption of linear elasticity has to be modified for finite displacements.

References


Figure 3: Numerical results for the second experiment: specific discharge \( q \), cation flux \( q^+ \), anion flux \( q^- \), displacement \( u \), fixed charge concentration \( c^f \), pressure \( p \).


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