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Kamyar Malakpoor

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Of one Essence is the human race
Thusly has Creation put the Base
One Limb impacted is sufficient
For all Others to feel the Mace

Saadi Shirazi, (1200 - 1292 CE)
Persian poet, prose writer and thinker.

Dedicated to my parents for the priceless gift
of their unconditional love and
of course
to my lovely sister.

Preface

After four degrees, at four universities, in three disciplines, I have learned one thing. I could never have done *any* of this, particularly the research and writing that went into this dissertation, without the support and encouragement of a lot of people.

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Eindhoven, February 2007 Kamyar Malakpoor

Contents

Nomenclature

Notations

a	scalar
$\mathbf{a}$, $\mathfrak{a}$	vector
A	scalar
$\mathbb{A}$	bilinear form
$\mathbf{A}$, $\mathfrak{A}$	matrix
$\boldsymbol{\mathcal{A}}$	tensor
$\boldsymbol{\mathcal{A}} : \boldsymbol{\mathcal{B}}$	$\mathrm{tr}(\boldsymbol{\mathcal{A}}\boldsymbol{\mathcal{B}}^T)$

Symbols

c	molar concentration of the fluid phase	[mol m^{-3}]
c^β	molar concentration of ion β per unit fluid volume	[mol m^{-3}]
c^{fc}	molar concentration of fixed charges attached to the solid skeleton per unit fluid volume	[mol m^{-3}]
$\boldsymbol{\mathcal{C}}$	right Cauchy-Green strain tensor	[-]
$\boldsymbol{\mathcal{D}}^\beta$	diffusivity of ion β	[m^2 s^{-1}]
$\boldsymbol{\mathcal{E}}$	Green strain tensor	[-]
f^β	activity coefficient of ion β	[-]
F	Faraday's constant	[C mol^{-1}]
$\boldsymbol{\mathcal{K}}$	hydraulic permeability	[m^4 N^{-1} s^{-1}]
$\boldsymbol{\mathcal{K}}^\beta$	chemical potential tensor per unit mixture volume for the β constituent	[N m^{-2}]
p	pressure of the fluid phase	[N m^{-2}]

$\mathbf{q}^l$	specific discharge relative to the solid	[m s^{-1}]
$\mathbf{q}^\beta$	flux of ion β relative to the fluid	[mol m^{-2} s^{-1}]
$\mathbf{q}^\beta_{\text{tot}}$	$\mathbf{q}^\beta + c^\beta \mathbf{q}$, total flux of ion	[mol m^{-2} s^{-1}]
R	universal gas constant	[J mol^{-1} K^{-1}]
$\boldsymbol{\mathcal{S}}$	second Piola-Kirchhoff stress	[N m^{-2}]
t	time	[s]
T	absolute temperature	[K]
$\mathbf{u}$	displacement	[m]
$\mathbf{v}^\alpha$	velocity of the α-phase	[m s^{-1}]
$\mathbf{v}^\beta$	velocity of ion β	[m s^{-1}]
$\mathbf{v}$	velocity of mixture	[m s^{-1}]
$\overline{V}^\beta$	partial molar volume of ion β	[m^3 mol^{-1}]
W	Helmholtz free energy	[J m^{-3}]
W_E	elastic energy	[J m^{-3}]
z^β	valance of ion β	[-]
z^{fc}	valance of fixed charge	[-]

Greek symbols

Γ^β	osmotic coefficient of ion β	[-]
λ_s	Lamé stress constant	[N m^{-2}]
μ^l	electro-chemical potential of the fluid phase	[N m^{-2}]
μ^β	electro-chemical potential of ion β	[J mol^{-1}]
$\tilde{\mu}^\beta$		[J m^{-3}]
μ_s	Lamé stress constant	[N m^{-2}]
π^α	momentum interaction with constituent other than α	[N m^{-3}]
$\boldsymbol{\Pi}$	first Piola-Kirchhoff stress	[N m^{-2}]
ρ^α	bulk density of the α-phase	[kg m^{-3}]
ρ^α_T	true density of the α-phase	[kg m^{-3}]
$\boldsymbol{\sigma}^\alpha$	partial stress tensor of constituent α	[N m^{-2}]
$\boldsymbol{\sigma}$	Cauchy stress tensor	[N m^{-2}]
φ^α	volume fraction of the α-phase	[-]
φ^β	volume fraction of the component β	[-]
Φ^β	volume fraction per unit initial volume	[-]
ξ	voltage	[V]
ψ^α	Helmholtz free energy of constituent β per unit volume mixture	[J m^{-3}]
Ψ^α	Helmholtz free energy of constituent β per unit volume constituent	[J m^{-3}]

Mathematical symbols and function spaces

Ω^α	:=	current configuration of the α-th constituent
Ω_0^α	:=	reference configuration of the α-th constituent
Ω	:=	domain
n	:=	dimension of Ω (2 or 3)
$\mathbf{x}$	:=	vector in current configuration
$\mathbf{X}$	:=	vector in reference configuration
∇	:=	gradient operator in current configuration, $\frac{\partial}{\partial \mathbf{x}}$
∇_0	:=	gradient operator in initial configuration $\frac{\partial}{\partial \mathbf{X}}$
Γ	:=	polygonal (polyhedral) boundary of Ω partitioned into non-empty Dirichlet and closed Neumann parts.
$\mathbf{n}(\mathbf{x})$	:=	outward unit normal vector from Ω at $\mathbf{x}$
$L^2(\Omega)$	:=	$\{f : \Omega \to \mathbb{R} : \ \|f\|_0 < \infty\}$
$\|f\|_0^2$	:=	$\int_\Omega \|f\|^2 \, d\mathbf{x}$
$\mathbf{L}^2(\Omega)$	:=	$\{\mathbf{f} : \Omega \to \mathbb{R}^n : \ \|\mathbf{f}\|_0 < \infty\}$
$\|\mathbf{f}\|_0^2$	:=	$\int_\Omega \|\mathbf{f}\|^2 \, d\mathbf{x}$
$D^\alpha v$	:=	$\dfrac{\partial^{\|\alpha\|} v}{\partial x_1^{\alpha_1} \cdots \partial x_n^{\alpha_n}}, \quad \alpha = (\alpha_1, \cdots, \alpha_n) \in \mathbb{N}^n$ with $\|\alpha\| = \sum_{i=1}^n \alpha_i$
$H^k(\Omega)$	:=	$\left\{v \in L^2(\Omega) : \ D^\alpha v \in L^2(\Omega) \quad \text{for all } \|\alpha\| \le k\right\}$
$C_0^\infty(\Omega)$	:=	space of all infinitely differentiable scalar functions $\varphi : \Omega \to \mathbb{R}$ with compact support in Ω
$H_0^k(\Omega)$	:=	closure of C_0^∞ in $H^k(\Omega)$
$\|v\|_k$	:=	$\sum_{\|\alpha\|=k} \|D^\alpha v\|_0$
$H^{-k}(\Omega)$	:=	the dual of $H^k(\Omega)$
$\gamma_D \phi$	:=	$\phi\|_\Gamma$, trace of a $H^1(\Omega)$ function
$H^{1/2}(\Gamma)$	:=	$H^{1/2}(\Gamma) = \left\{\gamma_D \varphi : \varphi \in H^1(\Omega)\right\}$
$\nabla\cdot$	:=	divergence operator in the current configuration
$\nabla_0\cdot$	:=	divergence operator in the reference configuration
$H(\mathrm{div};\Omega)$	:=	$\{\mathbf{q} \in \mathbf{L}^2(\Omega) : \ \nabla \cdot \mathbf{q} \in L^2(\Omega)\}$
$(\mathbf{q}_1, \mathbf{q}_2)_{\mathrm{div};\Omega}$	:=	$\int_\Omega \left(\mathbf{q}_1 \cdot \mathbf{q}_2 + \nabla \cdot \mathbf{q}_1 \nabla \cdot \mathbf{q}_2\right) \, d\mathbf{x}$
$\|\mathbf{q}\|_{\mathrm{div};\Omega}$	:=	$(\mathbf{q}, \mathbf{q})_{\mathrm{div};\Omega}^{1/2}$
$\gamma_N \mathbf{q}$	:=	$\mathbf{n} \cdot \mathbf{q}$, trace of a $H(\mathrm{div};\Omega)$ function
$H^{-1/2}(\Gamma)$	:=	$\{\gamma_N \mathbf{q} : \mathbf{q} \in H(\mathrm{div};\Omega)\}$
$\mathcal{V}$	:=	$\left\{\mathbf{u} \in (H^1(\Omega))^n : \mathbf{u} = 0 \text{ on } \Gamma_{\mathbf{u}}^D\right\}$
$H_D^1(\Omega)$	:=	$\left\{\varphi \in H^1(\Omega) : \varphi = 0 \text{ on } \Gamma_p^D\right\}$
$H_D^{1/2}(\Gamma)$	:=	$\left\{\lambda \in H^{1/2}(\Gamma) : \lambda = 0 \text{ on } \Gamma_p^D\right\}$
$H_N(\mathrm{div};\Omega)$	:=	$\left\{\mathbf{q} \in H(\mathrm{div};\Omega) : \mathbf{n} \cdot \mathbf{q} = 0 \text{ on } \Gamma_p^N\right\}$
$H_N^{-1/2}(\Gamma)$	:=	$\left\{\mu \in H^{-1/2}(\Gamma) : \mu = 0 \text{ on } \Gamma_p^N\right\}$
$\|\|\|(\mathbf{u}, \mathbf{q})\|\|\|_1$	:=	$\left(\|\mathbf{u}\|_1^2 + \|\mathbf{q}\|_{\mathrm{div};\Omega}^2\right)^{1/2}$
$\mathcal{T}_h$	:=	a triangulation of $\overline{\Omega}$

$$
\begin{array}{lcl}
H(\mathrm{div};\mathcal{T}_h) & := & \{\mathbf{q}\in\mathbf{L}^2(\Omega):\ \mathbf{q}|_T\in H(\mathrm{div};T)\ \text{ for all } T\in\mathcal{T}_h\}\\
\|\mathbf{q}\|_{\mathrm{div};\mathcal{T}_h} & := & \left(\|\mathbf{q}\|_0^2+\sum_{T\in\mathcal{T}_h}\|\nabla\cdot\mathbf{q}|_T\|_2^2\right)^{1/2}\\
P^k(T) & := & \text{the space of polynomials of degree}\le k\\
R^k(\partial T) & := & \{\varphi\in L^2(\partial T):\ \varphi|_F\in P^k(F)\quad\text{for all } F\subset\partial T\}\\
RT^k(T) & := & \{\boldsymbol{\phi}+q\mathbf{x}:\ \mathbf{x}\in T\text{with }\boldsymbol{\phi}\in(P^k(T))^n\text{ and }q\in P^k(\partial T)\}\\
\hat{T} & := & \left\{\hat{\mathbf{x}}=\sum_1^L\zeta_\ell\hat{\mathbf{x}}_\ell:0\le\zeta_\ell\le 1,\ \sum_1^L\zeta_\ell=1\right\}\\
P^1_{-1}(\mathcal{T}_h) & := & \{\varphi\in L^2(\Omega):\varphi|_T\in P^1(T)\ \text{ for all }\ T\in\mathcal{T}_h\}\\
P^1_0(\mathcal{T}_h) & := & P^1_{-1}(\mathcal{T}_h)\cap H^1(\Omega)\\
P^1_D(\mathcal{T}_h) & := & \{\varphi\in P^1_0(\mathcal{T}_h):\varphi=0\ \text{ on }\Gamma^D_{\mathbf{u}}\}\\
RT^0_{-1}(\mathcal{T}_h) & := & \{\mathbf{u}\in\mathbf{L}^2(\Omega):\ \mathbf{u}|_T\in RT^0(T)\ \text{ for all } T\in\mathcal{T}_h\}\\
RT^0_0(\mathcal{T}_h) & := & RT^0_{-1}(\mathcal{T}_h)\cap H(\mathrm{div};\Omega)\\
RT^0_{0,N}(\mathcal{T}_h) & := & RT^0_{-1}(\mathcal{T}_h)\cap H_N(\mathrm{div};\Omega)\\
\mathcal{E}_h & := & \text{the collection of edges } (n=2)\text{ or faces } (n=3)\text{ of sub-domains}\\
 & & T\in\mathcal{T}_h\\
M^0_{-1}(\mathcal{T}_h) & := & \{\lambda\in L^2(\Omega):\lambda|_T\in M^0(T)\ \text{ for all } T\in\mathcal{T}_h\}\\
\mathcal{E}_h^{\partial} & := & \{e\in\mathcal{E}_h:e\subset\Gamma\}\\
L^2(\mathcal{E}_h) & := & \prod_{T\in\mathcal{T}_h}L^2(\partial T)\\
M^0_{-1}(\mathcal{E}_h) & := & \{\lambda=(\lambda_e)_{e\in\mathcal{E}_h}\in H^{1/2}(\bigcup_{e\in\mathcal{E}_h}e):\lambda_e\in M^0(e)\text{ for all }\ e\in\mathcal{E}_h\}\\
M^0_{-1,D}(\mathcal{E}_h) & := & \{\lambda\in M^0_{-1}(\mathcal{E}_h):\lambda=0\quad\text{on}\quad\Gamma^D_p\}\\
M^0_{-1,l}(\mathcal{E}_h) & := & \{\lambda\in M^0_{-1}(\mathcal{E}_h):\lambda=\tilde{\mu}^l_{in}\quad\text{on}\quad\Gamma^D_p\}\\
M^0_{-1,\beta}(\mathcal{E}_h) & := & \{\lambda\in M^0_{-1}(\mathcal{E}_h):\lambda=\tilde{\mu}^\beta_{in}\quad\text{on}\quad\Gamma^D_p\},\ \beta=+,-
\end{array}
$$

Superscripts and Subscripts

D	Dirichlet boundary	0	reference state
N	Neumann boundary	h	discrete space variable
fc	fixed charge	n	discrete time variable
l	liquid	p	pressure
f	fluid	$\mathbf{u}$	displacement
s	solid	s	solid
$+$	cation		
$-$	anion		

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Chapter 1

Introduction

Intervertebral discs (or intervertebral fibrocartilage) are cartilaginous tissues that lie between adjacent vertebrae in the spine. Each disc forms a cartilaginous joint to allow slight movement of the vertebrae, and acts as a ligament to hold the vertebrae together.

Disc diseases like degenerated discs, slipped discs, herniated discs are common terms often related to back pain, both the lower back and the neck.

The spinal column is made up of bones called vertebrae. Each vertebra has six joints; four at the back of the bones that allow and control spinal movement. These are called facet joints and are aligned vertically, parallel to the direction of the spine. The other two joints are at the top and bottom of the vertebrae themselves. These joints are horizontal joints in orientation and weight-bearing in function. Between each pair of the vertebrae is an intervertebral disc, except between the top two in the neck.

The discs become progressively smaller as you go up the spine. They change shape as they go up, simply because the bones also change shape. The combination of two vertebrae and an intervertebral disc is called motion segment.

The intervertebral disc functions to permit limited motion and flexibility, while maintaining segmental stability and absorbing and distributing external loads.

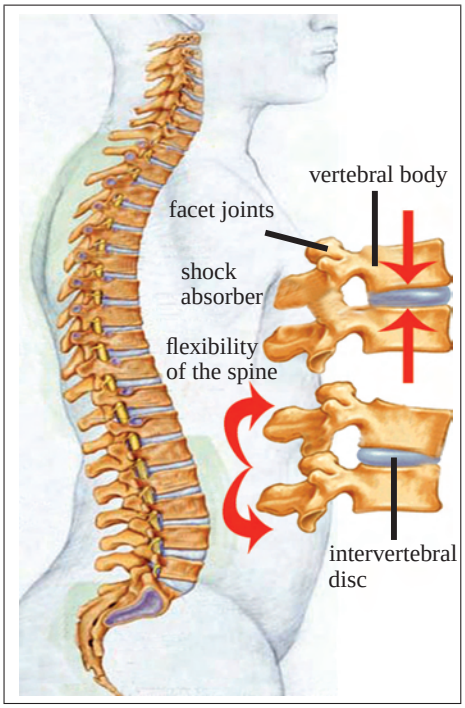

Figure 1.1. schematic of the spine and the motion segment

In fact, the intervertebral discs are fibrocartilaginous cushions serving as the spine's shock absorbing system, which protect the vertebrae, brain, and other structures (i.e. nerves). The discs allow some vertebral motion: extension and flexion. Individual disc movement is very limited period however considerable motion is possible when several discs combine.

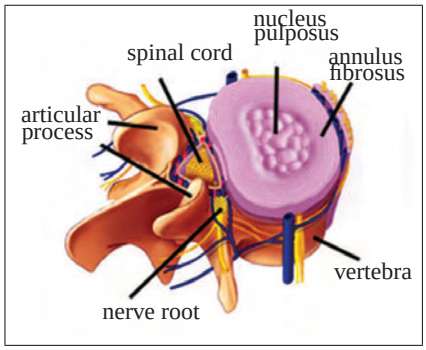

Figure 1.2. schematic representation of an intervertebral disc

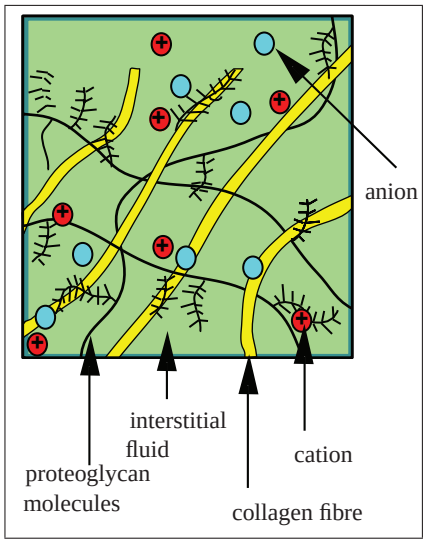

Figure 1.3. microscopic representation of an intervertebral disc

The structure of the normal intervertebral disc includes:

- A nucleus pulposus, soft and composed primarily of proteoglycans and Type II collagen with a capacity to absorb and distribute load.
- A tough outer annulus fibrosus with A well-organized layer of Type I collagen that serves to stabilize the motion segment.
- Two end plates that cover top and bottom of an intervertebral disc of type hyaline cartilage that allow fluid movement between disc and vertebral body.

The nucleus of the disc acts as a shock absorber, absorbing the impact of the body's daily activities and keeping the two vertebrae separated. The nucleus is roughly spherical in shape and is made of a hydrogel-like material. The weight of the body causes a considerable amount of pressure to be built up in the nucleus.

The annulus is wrapped in layers around the nucleus to contain its pressure. These layers are somewhat like the layers of an onion. The fibres of one layer are at right angles to the next layer. These layers have to be tough and non-yielding; otherwise the soft nucleus would lose its shape and spill all over the place.

In fact, the intervertebral disc can be likened to a doughnut: whereby the annulus fibrosis is similar to the dough and the nucleus pulposus is the jelly. If one presses down on the front of the doughnut the jelly moves posteriorly or to the back.

As people age, the nucleus pulposus begins to dehydrate, which limits its ability to absorb shock. The annulus fibrosus gets weaker with age and begins to tear. While this may not cause pain in some people, in others one or both of these may cause chronic pain.

Historically, Hippocrates (460-390 BC) is the father of spine surgery (Marketos and Skiadas, 1999a). Galen (129-210 AD) compiled treaties of orthopedic treatments like: experimental physiologist and made many true observations on how the body works. Galen described four spinal suffering, kyphosis, lordosis, scoliosis and seisis that occur due to tuberculosis nodes on the lungs, falls on to the hips or shoulders, aging and painful conditions (Marketos and Skiadas, 1999b).

The main structures of annulus fibrosus are a fibre network consist of collagen fibres and proteoglycan molecules, freely moving charged particles (Na^+ and Cl^-) and an interstitial fluid.

The large proteoglycan molecules consisting of a protein core to which up to 100 highly sulphated glycosaminoglycan chains (GAGs) are attached. A distinctive feature of glycosaminoglycan chains is their high number of charges. The concentration of these fixed charges is called the fixed charge density.
Because of the entanglement of the glycosaminoglycans in the collagen network, the charges of proteoglycans are fixed in the tissue, unlike the small ions like Na^+ and Cl^-.

The main function of the intervertebral disc is mechanical. The disc transmits load along the spinal column and also allows the spine to bend and twist. The loads on the disc arise from body weight and muscular activity, and change with posture.

Discs are under pressure, which varies with posture from around 0.1 to 0.2 MPa at rest, to around 1.5 to 2.5 MPa while bending and lifting. The pressure is mainly due to water pressure across the nucleus and inner annulus in a normal disc.

In fact, intervertebral discs exhibits swelling and shrinking behaviour which is caused by mechanical force(weight of the body), chemical force (changing the salt concentration) and electrical force (electrical potential field). In all cases the swelling is caused by inflow or outflow of fluid.

The fixed charge density is an important determinant of the swelling properties (osmotic pressure) of the intervertebral disc.

1.1 Existing models for swelling of intervertebral discs

Modelling the mechanical and electro-chemical behaviour of soft tissues such as intervertebral disc is an essential task in improving the understanding of failure mechanisms. Several researchers have posed sets of equations which present the mechanical and/or electro-chemical behaviour of such tissues.

We distinguish between the components and the phases in this way that the components are considered to be continua related to the same macroscopic volume measure for all components (in our case a solid, a liquid, anions, and cations), and phases are continua related to their own real volume measure (in our case solid and fluid). Mixture theory (Bowen, 1980) is a framework, in which the model integrates mechanical deformations and loads, diffusion, convection and chemical reactions of different solutes. Theories that describe the mechanical behaviour of cartilaginous tissues can be divided into three categories:

- An earlier study from geomechanics presents two-component models (biphasic), that describe the solid-fluid interactions.((Biot, 1941) and (Biot, 1972))

These models do not consider the electrical charge and therefore cannot describe osmotic effects, which have a major influence on the swelling behaviour of tissues.

- Osmotic effects are modelled in a triphasic model (Lai et al., 1991) and (Gu et al., 1997) that take into account the ionic effects. In the triphasic model three phases are defined: a charge porous solid phase (collagen fibers and proteoglycans), the interstitial fluid phase, and the fluid miscible phase (the ionic phase). The triphasic model extends the biphasic model using physico-chemical theory.

- In the four-component mixture theory (Huyghe and Janssen, 1997) a deformable and charged porous medium is saturated with a fluid with dissolved cations and anions. In fact, the four component model takes the geometric non-linearity, electrical fluxes and potential gradient into account. By introducing the electronegativity as a restriction on the second law of thermodynamics, electrical phenomena are modelled.

1.2 Finite element analysis for the numerical solution

The governing equations for the two-component model form a linear time-dependent system, involving solid displacement, fluid pressure and fluid flow.

In the case of a four-component model we are dealing with a nonlinear time-dependent system, involving solid displacement, liquid and ions potentials, liquid flow and ions flow, 15 equations and unknowns in a three-dimensional configuration.

Of the various forms of discretisation which are possible, one of the most used is the finite difference process. Another method that is often used in many physical applications is concerned with various trial function approximations falling under the general classification of finite element methods. It has been shown that even finite difference processes can be included as a subclass of this more general theory (Ciarlet, 1978).

The name “mixed method” is applied to a variety of finite element methods that have more than one approximation space. Typically one or more of the spaces play the role of Lagrange multipliers to enforce constraints. The name and many of the original concepts for such methods originated in solid mechanics where it was desirable to have a more accurate approximation of certain derivatives of displacement. However, for the Stokes equations that govern viscous fluid flow, the natural Galerkin approximation is a mixed method (Brezzi, 1974), (Fortin, 1977) and (Brezzi and Fortin, 1991).

In fact, mixed method involves the independent interpolation of a kinematic quantity, such as displacement, and a kinetic one, such as flow. Hybridization is a special class of mixed method. In fact, it is differentiated from mixed method because the kinetic variables are forced to satisfy an equilibrium relation. Because of the additional interpolation of the kinetic variable, mixed and hybrid methods generally require somehow more computational effort to implement at the element level than do standard methods. However this effort is well justified by the flexibility to spec-

ify independently the interpolation functions representing the kinetic variables within the element, as compared to conventional methods for which the kinetic variables are represented as derivatives of the kinematic ones.

1.3 Aims and contents of this thesis

In chapter 2 we give a historical overview of the mixture theory. Then step by step we construct the four-component mixture model for the swelling of tissues. We first present the kinematic consideration and the balance laws. Then the constitutive equations are derived. We present the set of field equations for the Lagrangian description for the four-component system. In some detail, the transformation of the equations to the reference configuration of the skeleton is discussed. The infinitesimal deformation assumption for the solid skeleton simplifies the equations. It is shown that this model in the absence of ions reduces to a two-component system.

To verify the numerical solutions for this model we need to derive a set of analytical solutions for the reduced system of equations. Chapter 3 is devoted to this fact. We set ourselves the task of deriving a set of analytical solutions for the one-dimensional four-component model. We derive the analytical solutions for the two-component mixture model which is simpler and then generate the solution for the four-component model.

In chapter 4, the two-component model is considered. In our model it is desirable to obtain approximations of the fluid flow and ions flow that fulfil the conservation equations. In finite element simulations, these quantities are generally calculated by differentiation of the electro-chemical potential solutions. This approach may lead to violation of the mass conservation principle. We propose a mixed formulation for the two-component mixture. The existence and uniqueness for the solution of the discretised system is proven. We introduce the mixed hybrid technique. Although the hybridization method reduces the number of degrees of freedom, in the computations we only have to compute inverses of element-wise block diagonal matrices. The derived algorithms are tested for two type of examples: a one-dimensional consolidation experiment and a two-dimensional footing problem. The results for the first problem is verified with the analytical solutions derived in chapter 3.

In chapter 5, the mixed variational formulation for the four-component model is considered. The existence and uniqueness after discretisation in space and time for the solution of the linearised system is proven. Using the MHFEM technique for our model, we still have an indefinite system but the advantage is that the number of degrees of freedom will be reduced. In fact, for a three-dimensional problem this number will be reduced from 15 to 6 degrees of freedom.

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Chapter 2

Thermodynamic modelling of deformable saturated porous media[⋆]

In many branches of engineering, for example, in chemical engineering, material science, and soil mechanics, as well as in biomechanics, the reactions of material systems undergoing external or internal loading must be studied and described precisely in order to be able to predict the responses of these systems. Subsequently, the most important point of the investigation is to determine the composition of the body, because one must know the physically and chemically differing materials that constitute the system under consideration. The material systems in these fields of engineering can be composed in various ways. Solids can contain closed and open pores. The pores can be filled with fluids and, due to the material properties of the solids and the motions of the fluids, there are maybe interaction between the constituents.

Because the exact description of the locations of the pores (empty or filled with fluids) and the solid material is practically impossible, the heterogeneous composition can be investigated using the volume fraction concept. This concept results in the effect that "smeared" substitute continua with reduced densities for the solid and fluid phases arise which can then be treated by the mixture theory.

Reflections on the fundamentals of mechanics, which were already formulated to a great extent in the eighteenth and nineteenth centuries, have been considered in the last decades, beginning in the 1950s. These results form the basis of modern continuum mechanics, which makes a consistent treatment of gaseous, liquid, and solid bodies possible. Modern continuum mechanics was essentially formed by Truesdell. In two books (Truesdell and Toupin, 1960) and (Truesdell and Noll, 1965) and in numerous articles, he and his disciples laid down their ideas and created a closed continuum theory. However, their work is not undisputed.

Moreover, Truesdell was the scientist who reformulated and extended the mixture theory. After the fundamental work of Stefan, Duhmen, Gibbs, Raynolds, Jaumann, and Lohr, it was Truesdell (Truesdell, 1957) who introduced local balance equations

[⋆] Parts of this chapter will be appeared in ESAIM: Mathematical Modelling and Numerical Analysis (Malakpoor et al., 2006)

for mass, momentum, and energy of arbitrary constituted mixtures. These balance equations are referred to the individual constituents in consideration of all coupling terms. Truesdell used as a basis of his derivations certain principles, which later have been adopted as so-called "metaphysical principles":

1 All properties of the mixture must be mathematical consequences of properties of the constituents.

2 So as to describe the motion of a constituent, we may in imagination isolate it from the rest of the mixture, provided we allow properly for the actions of the other constituents upon it.

3 The motion of the mixture is governed by the same equations as is a single body.

In Truesdell's description of mixtures (Truesdell and Toupin, 1960), both a proper statement for the moment of momentum balance equation and a generalization of the entropy inequality for mixtures were missing. With respect to Truesdell's mixture theory, (Kelly, 1964) developed distinct balance laws on the basis of one fundamental balance equation, thus allowing a clear assignment of the effects resulting from the partial balance equations to the mechanical quantities of the mixture. Concerning the moment of momentum balance, Kelly proposed moment of momentum supply terms, thus admitting unsymmetrical partial stress tensors.

In the early 1960s, a thermodynamic approach to the constitutive theory was generally unknown, until (Coleman and Noll, 1963) as well as (Coleman and Mizel, 1964) introduced the development of thermodynamic restrictions from the entropy inequality. This application of the entropy inequality to heterogeneous materials caused exceptional difficulties.

It was later pointed out that the entropy inequality postulated by (Bowen, 1967) was the first correct version of the entropy inequality for mixtures. The development of the mixture theory was brought to an end to a certain extent already in the early 1970s, namely in so far as the fundamentals developed up to that time have remained valid up to today.

In the theory of mixtures (Bowen, 1976), one porous solid skeleton and $k-1$ miscible or immiscible pore-fluids are considered. The motivations and examples of mixtures can be found in many branches of science and engineering, like the investigation of the coupled solid deformation and pore-fluid flow behaviour in geoscience, the well-known consolidation problem of soil mechanics, in applications concerning the exploitation of natural gas and oil reservoirs, or in biomechanical problems like the investigation of swelling and shrinking of cartilaginous tissues or intervertebral disks, which is the main item of this work. For the case of saturated porous media, the main idea is the representation of a saturated porous medium as the superposition, in time and space, of two continua or phases; the first representing the skeleton phase, the second the fluid phase. The fluid volume fraction of a given volume is the ratio of the non-solid volume to the total volume and is denoted by φ^f.

As mentioned above, in the theory of mixture there is no measure to get any microscopic information. Therefore it is convenient to combine the theory of mixtures

with the concept of volume fractions. By this procedure, basically defining the theory of porous media, one can find an excellent tool for the description of general immiscible multiphasic aggregates, where the volume fractions are the measures of the local portions of the individual phases of the overall medium.

It seems that Morland (Morland, 1972) was the first scientist to use the volume fraction concept in connection with the mixture theory. In 1966, however, Mills (Mills, 1966) had already used the volume fraction concept for incompressible mixtures of two separated Newtonian fluids. In this article, Mills also formulated the incompressibility condition in such a way that he assumed the real densities of both constituents to be constant, i.e., that the sum of the volume fractions was equal to one. In the volume fraction concept, it is assumed that the porous solid always models a control space and that only liquids contained in the pores can leave the control space.

The basis of the description of porous media, using elements of the theory of mixtures restricted by the volume fraction concept, is the model of a macroscopic body, where neither a geometrical interpretation of the pore structure nor the exact location of the individual components of the body (constituents) are considered (Ehlers, 2002), (Hassanizadeh, 1986a) and (Hassanizadeh, 1986b). We proceed from the assumption that the constituents are "smeared" over the control space that is shaped by the porous solid, i.e., that each substitute constituent occupies the total volume of space simultaneously with the other constituents.

In this chapter, we consider a continuously deformable saturated porous medium. This type of saturated porous media can be observed in numerous solid mechanics problems and is studied since many years in civil engineering. It is also studied in biomechanics to model the coupling between fluid flow and mechanical loading in cartilage or skin.

Many biological porous media exhibit swelling and shrinking behaviour when in contact with salt concentrations. This phenomenon, observed in cartilage and gels, is caused by electric charges fixed to the solid, counteracted by corresponding charges in fluid. These charges result in a variety of features, including swelling, electro-osmosis, streaming potentials and streaming currents. We distinguish between the components and the phases in this way that the components are considered to be continua related to the same macroscopic volume measure for all components (in our case a solid, a fluid, anions, and cations), and phases are continua related to their own real volume measure (in our case solid and fluid). Mixture theory (Bowen, 1980) is a framework, in which the model integrates mechanical deformations and loads, diffusion, convection and chemical reactions of different solutes.

An earlier study from geomechanics presents biphasic models, that describe the solid-fluid interactions. These models can not describe osmotic effects, which have a major influence on the behaviour of tissues. Osmotic effects are modelled in a triphasic model (Lai et al., 1991) and (Gu et al., 1997) and in a four-component mixture theory (Huyghe and Janssen, 1997), (Frijns, 2001) and (Chen et al., 2006). In the four-component mixture theory a deformable and charged porous medium is saturated with a fluid with dissolved cations and anions.

The solid skeleton and fluid are assumed to be intrinsically incompressible and therefore a non-zero fluid flux divergence gives rise to swelling or shrinkage of the porous medium. Alternatively, a gradient in fluid pressure, ion concentrations or

voltage results in flow of the fluid and ions (Frijns, 2001).

In this chapter, we construct the model of four-component porous material in Lagrangian coordinates of the skeleton. Such a description, particularly useful in computer-aided solutions, has not been used yet for multi-phase systems where the skeleton is usually described in Eulerian coordinates.

This chapter is outlined as follows. In the next two sections, we present the kinematic consideration and the balance laws. Section 3 is devoted to constitutive equations. In section 4 we present the set of field equations for the Lagrangian description for the four-component system. In some detail, the transformation of the equations to the reference configuration of the skeleton is discussed. The sixth section is devoted to the Donnan equilibrium and boundary conditions. In section 7 we assume an infinitesimal deformation for the solid skeleton and we derive the simplified equations. In section 8 we present the reduction to a two-component system.

2.1 Kinematic

The swelling and shrinking behaviour of cartilaginous tissues (like intervertebral disc) can be modelled by a four- component mixture theory in which a deformable and charged porous medium is saturated with a fluid with dissolved ions. Within the concept of mixture theory, we consider a porous solid skeleton and an immiscible pore-fluid. The idea is to present the saturated porous medium as a superposition of deformable phases that occupy the same domain in the three-dimensional space at time t. In other words, we assume that different phases exist simultaneously at each point in space. Cartilaginous tissues are assumed to consist of two phases, a solid phase and a fluid phase. In cartilaginous tissues, the fluid phase consists of three components: liquid, cation and anion. We use the abbreviation s and f respectively for the solid phase and the fluid phase. The symbols l, $+$ and $-$ stand for liquid, cation and anion, respectively (cf. Figure 2.1).

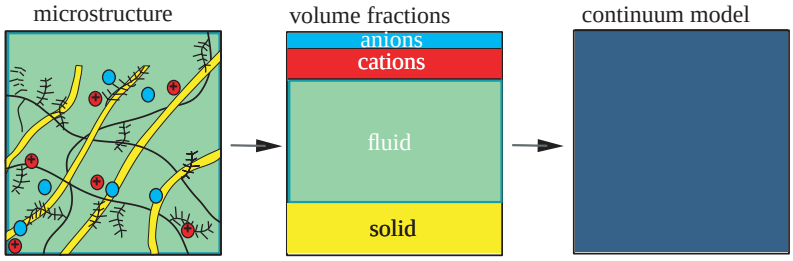

Figure 2.1. Micro-structure and macroscopic model

Definition 2.1. *A body $\mathcal{Q}$ is a set whose elements can be put into bijective correspondence with the points of a region Ω of a Euclidean point space. The elements of Ω are called particles and Ω is referred to as a configuration of $\mathcal{Q}$; the point in Ω to which a given particle of $\mathcal{Q}$ corresponds is said to be occupied by that particle.*

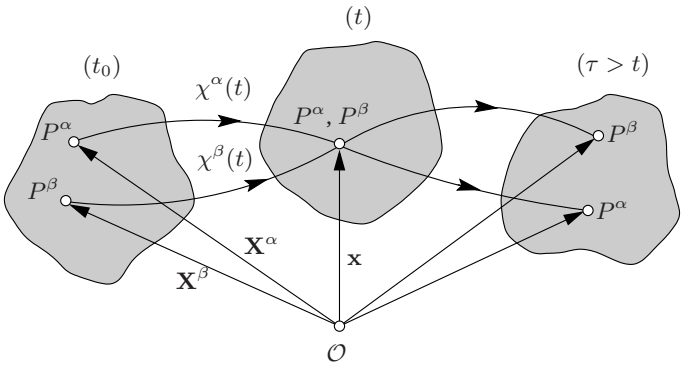

Figure 2.2. Motion of a multi-component mixture.

Definition 2.2. *A mixture can be considered as a superposition of deformable phases, that occupy the same domain in the three-dimensional space at time t.*

In order to represent the motion of the mixture, quantities associated with the motions of the phases and the mixture as a whole must be defined.

Definition 2.3. *Consider a porous media with the constituents $\alpha = s, l, +$ and $-$. Let Ω^α denotes the current configuration of the α-th constituent, whose domain Ω^α and boundary Γ^α are shared with other phases at time t. The kinematics in porous media theory are based on two fundamental assumptions:*

1 *The regions Ω^α coincide and every position $\mathbf{x}$ is occupied by particles of every single constituent at the same time.*

2 *Each constituent follows an independent motion and has a fixed but otherwise arbitrary reference configuration Ω_0^α occupying a domain Ω_0^α at time t_0.*

Define the motion

$$\mathbf{x} = \chi^\alpha(\mathbf{X}^\alpha, t) : \Omega^\alpha \times [0, T] \to \Omega,\ \alpha = s, l, +, -, \tag{2.1.1}$$

where $\mathbf{X}^\alpha$ is the position of the particle of the α-th constituent in its reference configuration, t is the time and $\mathbf{x}$ is the spatial position occupied at time t by the particle labeled by $\mathbf{X}^\alpha$.

As illustrated in Figure 2.2, each spatial point $\mathbf{x}$ of the current configuration is, at any time t, simultaneously occupied by material particles (material points) P^α. These particles proceed from different reference positions at time t_0, thus, each phase is assigned to its own motion function as mentioned above. As a result, each spatial point $\mathbf{x}$ can only be occupied by one single material point P^α of each phase. The function χ^α is the deformation function and the assumption of unique motion functions, where each material point P^α of the current configuration has a unique reference position $\mathbf{X}^\alpha$ at time t_0, requires the existence of the unique inverse motion function $(\chi^\alpha)^{-1}$.

Define the deformation gradient of the solid phase by

$$\boldsymbol{\mathcal{F}}^s(\mathbf{X}^s,t)=\nabla_{\mathbf{X}^s}\chi^s=\frac{\partial\chi^s}{\partial\mathbf{X}^s},\quad(\boldsymbol{\mathcal{F}}^s)^{-1}(\mathbf{x},t)=\nabla_{\mathbf{x}}(\chi^s)^{-1}=\frac{\partial\mathbf{X}^s}{\partial\mathbf{x}}. \tag{2.1.2}$$

A transfer from the current configuration to the reference configuration is possible by using the determinant of the gradient deformation as defined by

$$J^s(\mathbf{X}^s,t)=\det\boldsymbol{\mathcal{F}}^s>0. \tag{2.1.3}$$

Define the right Cauchy-Green strain tensor $\boldsymbol{\mathcal{C}}$ and Green strain tensor $\boldsymbol{\mathcal{E}}$ by

$$\boldsymbol{\mathcal{C}}(\mathbf{X}^s,t) = (\boldsymbol{\mathcal{F}}^s)^T\boldsymbol{\mathcal{F}}^s, \tag{2.1.4}$$

$$\boldsymbol{\mathcal{E}}(\mathbf{X}^s,t) = \frac{1}{2}(\boldsymbol{\mathcal{C}}-\boldsymbol{\mathcal{I}}). \tag{2.1.5}$$

Easily it can be seen that $\boldsymbol{\mathcal{E}}$ is symmetric positive definite.

Definition 2.4. *The true density for the α-constituent is defined as the mass of the α-constituent per unit volume of the α-constituent and is denoted by ρ^α_T. The bulk density ρ^α is the mass of the α-constituent per unit volume of the mixture. The quantity*

$$\varphi^\alpha(\mathbf{x},t)=\frac{\rho^\alpha(\mathbf{x},t)}{\rho^\alpha_T(\mathbf{x},t)}, \tag{2.1.6}$$

is called the volume fraction of the α-constituent. Physically φ^α represents the volume of the α-th constituent per unit volume of the mixture.
The velocity of $\mathbf{X}^\alpha$ is defined by

$$\mathbf{v}^\alpha=\frac{\partial\chi^\alpha}{\partial t}(\mathbf{X}^\alpha,t). \tag{2.1.7}$$

The density of the fluid phase is defined by

$$\rho^f=\sum_{\beta=l,+,-}\rho^\beta. \tag{2.1.8}$$

The velocity of the fluid $\mathbf{v}^f$ is defined by

$$\mathbf{v}^f=\frac{1}{\rho^f}\sum_{\beta=l,+,-}\rho^\beta\mathbf{v}^\beta. \tag{2.1.9}$$

The density of the mixture is defined by

$$\rho=\sum_{\alpha=s,l,+,-}\rho^\alpha. \tag{2.1.10}$$

The velocity of the mixture $\mathbf{v}$ *is defined by*

$$\mathbf{v} = \frac{1}{\rho} \sum_{\alpha=s,l,+,-} \rho^{\alpha} \mathbf{v}^{\alpha}. \tag{2.1.11}$$

If Ψ *is any scalar function of* $\mathbf{x}$ *and* t*, the derivatives of* Ψ *following the motion generated by* $\mathbf{v}$ *and* $\mathbf{v}^{\alpha}$ *are, respectively,*

$$\frac{D\Psi}{Dt} = \frac{\partial \Psi}{\partial t} + \nabla \Psi \cdot \mathbf{v}, \tag{2.1.12}$$

$$\frac{D^{\alpha}\Psi}{Dt} = \frac{\partial \Psi}{\partial t} + \nabla \Psi \cdot \mathbf{v}^{\alpha}. \tag{2.1.13}$$

2.2 Balance equations

In mixture theory and porous media theory, balance equations like balance of mass, balance of momentum, and moment of momentum, as well as balance of energy must be established for each constituent in consideration of all interactions and external agencies. This means that all quantities resulting from long- and short-range effects that influence the individual constituents, as well as the interaction effects between the constituents, have to be considered in the balance equations.

Before stating the balance and constitutive equations in the next section, we consider the following assumptions:

1. The mixture is incompressible, which means that both fluid and solid are incompressible. Hence ρ_T^s and ρ_T^f are uniform in position and constant in time. In other words, volumetric changes of the porous medium are taken into account.

2. We assume that no chemical reactions exist between phases and no sources or sinks exist.

3. We neglect the inertia effects and body forces.

4. The process are assumed to be isothermal.

5. The mixture is assumed to be saturated, i.e,

$$\boxed{\varphi^s + \varphi^f = 1.} \tag{2.2.1}$$

The volume fraction of the ions is neglected compared to those of the solid and the fluid (dilute solution),

$$\boxed{\varphi^+ + \varphi^- \approx 0 \Longrightarrow \varphi^f = \sum_{\beta=l,+,-} \varphi^{\beta} \approx \varphi^l.} \tag{2.2.2}$$

6. It is assumed that the solid matrix is entirely elastic and initially isotropic. The shear stress associated with mixture deformation is assumed to be negligible in the fluid phase. We assume that the porous medium is initially homogenous and therefore φ^s is initially uniform. For our binary porous medium $\varphi = \varphi^f \approx \varphi^l$ indicates porosity and note that $\varphi^s = 1 - \varphi$.

Conservation of mass for the phases s and f implies

$$\frac{\partial \varphi^\alpha}{\partial t} + \nabla \cdot (\varphi^\alpha \mathbf{v}^\alpha) = 0, \ \alpha = s, f. \tag{2.2.3}$$

Summing up these two equations for $\alpha = s, f$, and using the saturation assumption (2.2.1), the incompressibility constraint condition reads

$$\boxed{\nabla \cdot \left(\mathbf{q}^l + \mathbf{v}^s \right) = 0,} \tag{2.2.4}$$

where the specific discharge relative to the solid phase is defined by

$$\mathbf{q}^l = \varphi \left(\mathbf{v}^l - \mathbf{v}^s \right). \tag{2.2.5}$$

Note that the fluid velocity is a weighted average of the velocity of the liquid and the velocities of the ions. Since we are interested in the situation in which there are far more water molecules than ions, we approximate the velocity of the fluid by the velocity of the liquid, $\mathbf{v}^f \approx \mathbf{v}^l$.

The conservation of mass for the dissolved ions implies

$$\boxed{\frac{\partial \varphi c^\beta}{\partial t} + \nabla \cdot (\varphi c^\beta \mathbf{v}^\beta) = 0, \quad \beta = +, -,} \tag{2.2.6}$$

where c^β is the molar concentration of ion β per unit fluid volume and $\mathbf{v}^\beta$ is the average velocity of ion β. Define the molar flux $\mathbf{q}^\beta$ relative to the fluid with

$$\mathbf{q}^\beta = \varphi c^\beta (\mathbf{v}^\beta - \mathbf{v}^l). \tag{2.2.7}$$

After neglecting body forces and inertia effects, the momentum balance takes the form

$$\nabla \cdot \boldsymbol{\sigma}^\alpha + \boldsymbol{\pi}^\alpha = \mathbf{0}, \quad \alpha = s, l, +, -, \tag{2.2.8}$$

where $\boldsymbol{\sigma}^\alpha$ is the partial stress tensor of constituents α, $\boldsymbol{\pi}^\alpha$ is the momentum interaction with constituents other than α. The momentum balance for the mixture reads

$$\boldsymbol{\pi}^s + \boldsymbol{\pi}^l + \boldsymbol{\pi}^+ + \boldsymbol{\pi}^- = \mathbf{0}. \tag{2.2.9}$$

Hence

$$\boxed{\nabla \cdot \boldsymbol{\sigma} = \nabla \cdot \boldsymbol{\sigma}^s + \nabla \cdot \boldsymbol{\sigma}^l + \nabla \cdot \boldsymbol{\sigma}^+ + \nabla \cdot \boldsymbol{\sigma}^- = \mathbf{0},} \tag{2.2.10}$$

where $\boldsymbol{\sigma}$ represents the Cauchy stress tensor of the mixture.

The balance of moment of momentum requires that the stress tensor $\boldsymbol{\sigma}$ be symmetric. The partial stresses $\boldsymbol{\sigma}^\alpha$ are symmetric, if no moment of momentum interaction between constituents occurs (a proof can be found in (Bowen, 1976)). In this work we shall assume all partial stresses to be symmetric.

Electroneutrality requires

$$\boxed{z^+c^+ + z^-c^- + z^{fc}c^{fc} = 0,} \tag{2.2.11}$$

where z^β, $\beta = +, -$, is the valence of the dissolved ion β. For a mono-valent salt, $z^+ = 1$ and $z^- = -1$. The superscript fc stands for fixed charge, i.e. the attached ionic group, thus c^{fc} denotes the molar concentration of the ions attached to he solid skeleton per unit fluid volume.

The conservation of fixed charge reads

$$\boxed{\frac{\partial \varphi c^{fc}}{\partial t} + \nabla \cdot (\varphi c^{fc} \mathbf{v}^s) = 0.} \tag{2.2.12}$$

In order to gain restrictions for constitutive equations, the second law of thermodynamics (entropy inequality) has been usefully applied in continuum mechanics, in mixture theory and, in particular, in the theory of porous media. Following the isothermality and incompressibility conditions, the entropy inequality for a unit volume of the mixture reads (Bowen, 1976):

$$\sum_{\alpha=s,l,+,-} \left(-\varphi^\alpha \frac{D^\alpha \Psi^\alpha}{Dt} + \boldsymbol{\sigma}^\alpha : \nabla \mathbf{v}^\alpha - \boldsymbol{\pi}^\alpha \cdot \mathbf{v}^\alpha \right) \geq 0, \tag{2.2.13}$$

where Ψ^α is the free energy density for the α-constituent per unit volume of the α-th constituent and is defined by $\varphi^\alpha \Psi^\alpha = \psi^\alpha$, where ψ^α is the Helmholtz free energy of constituent α per unit mixture volume.

Define W to be the Helmholtz free energy of the mixture by

$$W = J^s \sum_{\alpha=s,l,+,-} \psi^\alpha = J^s \sum_{\alpha=s,l,+,-} \varphi^\alpha \Psi^\alpha. \tag{2.2.14}$$

We try to rewrite the entropy inequality (2.2.13) per initial mixture volume. Note that

$$\frac{D^s J^s}{Dt} = J^s \nabla \cdot \mathbf{v}^s. \tag{2.2.15}$$

Material time differentiation of W with respect to the solid motion gives

$$\frac{D^s W}{Dt} = W \nabla \cdot \mathbf{v}^s + J^s \sum_{\alpha=s,l,+,-} \frac{D^s \varphi^\alpha}{Dt} \Psi^\alpha + J^s \sum_{\alpha=s,l,+,-} \varphi^\alpha \frac{D^s \Psi^\alpha}{Dt}. \tag{2.2.16}$$

Evidently,

$$\frac{D^s\Psi^\alpha}{Dt} = \frac{D^\alpha\Psi^\alpha}{Dt} + \nabla\Psi^\alpha \cdot (\mathbf{v}^s - \mathbf{v}^\alpha), \tag{2.2.17}$$

so,

$$\begin{aligned} -J^s \sum_{\alpha=s,l,+,-} \varphi^\alpha \frac{D^\alpha\Psi^\alpha}{Dt} &= -\frac{D^sW}{Dt} + W\nabla\cdot\mathbf{v}^s \\ &+ J^s \sum_{\alpha=s,l,+,-} \frac{D^s\varphi^\alpha}{Dt}\Psi^\alpha \\ &- J^s \sum_{\beta=l,+,-} \varphi^\beta \nabla\Psi^\beta \cdot (\mathbf{v}^\beta - \mathbf{v}^s). \end{aligned}$$

The definition of the material time derivative in (2.1.13) and the incompressibility assumption (2.2.3) imply that

$$\begin{aligned} & J^s \sum_{\alpha=s,l,+,-} \frac{D^s\varphi^\alpha}{Dt}\Psi^\alpha \\ = \;& J^s \sum_{\alpha=s,f,+,-} \left(\Psi^\alpha \frac{\partial\varphi^\alpha}{\partial t} + \Psi^\alpha \nabla\varphi^\alpha \cdot \mathbf{v}^s \right) \\ = \;& J^s \sum_{\alpha=s,f,+,-} \left(\Psi^\alpha \frac{\partial\varphi^\alpha}{\partial t} + \Psi^\alpha \left(\nabla\cdot(\varphi^\alpha\mathbf{v}^s) - \varphi^\alpha\nabla\cdot\mathbf{v}^s\right) \right) \\ = \;& -J^s\nabla\cdot\mathbf{v}^s \sum_{\alpha=s,f,+,-} \Psi^\alpha\varphi^\alpha - J^s \sum_{\beta=l,+,-} \Psi^\beta \nabla\cdot\left(\varphi^\beta(\mathbf{v}^\beta - \mathbf{v}^s)\right) \\ + \;& J^s \sum_{\alpha=s,l,+,-} \Psi^\alpha \underbrace{\left(\frac{\partial\varphi^\alpha}{\partial t} + \nabla\cdot(\varphi^\alpha\mathbf{v}^\alpha) \right)}_{=0} \\ = \;& -W\nabla\cdot\mathbf{v}^s - J^s \sum_{\beta=l,+,-} \Psi^\beta \nabla\cdot\left(\varphi^\beta(\mathbf{v}^\beta - \mathbf{v}^s)\right). \end{aligned}$$

Thus

$$-J^s \sum_{\alpha=s,l,+,-} \varphi^\alpha \frac{D^\alpha\Psi^\alpha}{Dt} = \frac{D^sW}{Dt} - J^s \sum_{\beta=s,l,+,-} \nabla\cdot\left(\Psi^\beta\varphi^\beta(\mathbf{v}^\beta - \mathbf{v}^s)\right) \tag{2.2.18}$$

By using equations (2.2.8) and (2.2.10) we have

$$\sum_{\alpha=s,l,+,-} \boldsymbol{\sigma}^\alpha : \nabla\mathbf{v}^\alpha = \sum_{\alpha=s,l,+,-} \boldsymbol{\sigma}^\alpha \nabla\mathbf{v}^s + \sum_{\beta=l,+,-} \boldsymbol{\sigma}^\beta : \nabla(\mathbf{v}^\beta - \mathbf{v}^s)$$

$$
\begin{aligned}
&= \boldsymbol{\sigma}\nabla\mathbf{v}^s + \sum_{\beta=l,+,-} \nabla\cdot\Big(\boldsymbol{\sigma}^\beta(\mathbf{v}^\beta-\mathbf{v}^s)\Big)\\
&- \sum_{\alpha=s,l,+,-} \nabla\cdot\boldsymbol{\sigma}^\alpha\cdot\mathbf{v}^\alpha + \mathbf{v}^s \underbrace{\sum_{\alpha=s,l,+,-} \nabla\cdot\boldsymbol{\sigma}^\alpha}_{0}\\
&= \boldsymbol{\sigma}\nabla\mathbf{v}^s + \sum_{\beta=l,+,-} \nabla\cdot\Big(\boldsymbol{\sigma}^\beta(\mathbf{v}^\beta-\mathbf{v}^s)\Big) + \sum_{\alpha=s,l,+,-} \boldsymbol{\pi}^\alpha\cdot\mathbf{v}^\alpha,
\end{aligned}
\tag{2.2.19}
$$

therefore the entropy inequality with respect to the initial state of porous solid takes the following form

$$
\boxed{-\frac{D^sW}{Dt} + J^s\boldsymbol{\sigma} : \nabla\mathbf{v}^s - J^s\sum_{\beta=l,+,-}\nabla\cdot\Big(\boldsymbol{\mathcal{K}}^\beta\cdot(\mathbf{v}^\beta-\mathbf{v}^s)\Big)\geq 0.} \tag{2.2.20}
$$

where $\boldsymbol{\mathcal{K}}^\beta$ is the *chemical potential* tensor per unit mixture volume for the β-constituent and is defined by

$$
\boldsymbol{\mathcal{K}}^\beta = \psi^\beta\boldsymbol{\mathcal{I}} - \boldsymbol{\sigma}^\beta, \quad \beta = l,+,-. \tag{2.2.21}
$$

2.3 Constitutive equations

Mixture theory (the basis of porous media theory) is closed, i.e., the number of unknown fields is equal to the sum of the balance equations and the constitutive equations. In porous media theory, therefore, one has to look for additional equations in order to close the system of field equations by introducing constitutive equations. These equations connect certain mechanical or thermodynamical quantities via material-dependent constants and must be provided with a Lagrange multipliers for the evaluation in process of the entropy inequality. If the equation in excess is a constraint of the motion, then the Lagrange multiplier will become an unknown reaction force.

However, it is not sufficient to only fulfil the requirement. Rather more general "principles", which were developed in continuum mechanics should be fulfilled. They are:

- Principle of material frame-indifference or objectivity, or in some literature known as principle of change of observer. This principle states that the response of any material must be independent of the observer.
- Principle of dissipation. This principle states that the constitutive relations must satisfy the reduced entropy inequality (2.2.20) for all values of their arguments (Coleman and Noll, 1963).
- Principle of equipresence. (Truesdell and Toupin, 1960). This states that if a variable is used in one constitutive relation of a problem, it should be used in

all the constitutive relations for that problem (unless, its presence contradicts some other law or axiom).

Note that the entropy inequality should hold for all mixtures satisfying the balance laws, incompressibility and electro-neutrality.

Due to the objectivity principle, we refer the current description of the mixture to the initial state of the porous solid.

Defining volume fractions

$$\Phi^\alpha = J^s \varphi^\alpha, \quad \alpha = s, l, +, -, \tag{2.3.1}$$

per unit initial volume, we can rewrite the balance equation (2.2.3) as follows:

$$\frac{D^s \Phi^\alpha}{Dt} + J^s \nabla \cdot (\varphi^\alpha (\mathbf{v}^\alpha - \mathbf{v}^s)) = 0, \quad \alpha = s, l, +, -. \tag{2.3.2}$$

We shall denote Φ^f by Φ. By introducing a Lagrange multiplier p for the incompressibility constraint (2.2.4), the entropy inequality (2.2.20) takes the form

$$\begin{aligned} - & \frac{D^s W}{Dt} + J^s (\boldsymbol{\sigma} + p\boldsymbol{\mathcal{I}}) : \nabla \mathbf{v}^s + J^s (-\boldsymbol{\mathcal{K}}^l + p\varphi \boldsymbol{\mathcal{I}}) : \nabla (\mathbf{v}^l - \mathbf{v}^s) \\ - & J^s \sum_{\beta=+,-} \boldsymbol{\mathcal{K}}^\beta : \nabla (\mathbf{v}^\beta - \mathbf{v}^s) + J^s (-\nabla \cdot \boldsymbol{\mathcal{K}}^l + p \nabla \varphi) \cdot (\mathbf{v}^l - \mathbf{v}^s) \\ - & J^s \sum_{\beta=+,-} \nabla \cdot \boldsymbol{\mathcal{K}}^\beta \cdot (\mathbf{v}^\beta - \mathbf{v}^s) \geq 0. \end{aligned} \tag{2.3.3}$$

The electro-neutrality condition (2.2.11) in the initial state takes the following form

$$\Phi z^+ c^+ + \Phi z^- c^- + z^{fc} \varphi_0 c_0^{fc} = 0. \tag{2.3.4}$$

It is easy to check that

$$\frac{D^s \Phi c^\beta}{Dt} + J^s \nabla \cdot \Big(\varphi c^\beta (\mathbf{v}^\beta - \mathbf{v}^s) \Big) = 0, \quad \forall \beta = +, -. \tag{2.3.5}$$

After combining (2.3.4) and (2.3.5), we obtain another constraint for the entropy inequality as:

$$\boxed{\sum_{\beta=+,-} \frac{1}{\overline{V}^\beta} \nabla \cdot \Big(z^\beta \varphi^\beta (\mathbf{v}^\beta - \mathbf{v}^s) \Big) = 0.} \tag{2.3.6}$$

Here we use that

$$\overline{V}^\beta c^\beta = \frac{\varphi^\beta}{\varphi}, \quad \beta = l, +, -, \tag{2.3.7}$$

where $\overline{V}^\beta$ is the molar volume of the constituent β, $\beta = l, +, -$ and $c^l = c - c^+ - c^-$. Here c is the molar concentration of the fluid phase, which is assumed to be uniform and constant.

The equation (2.3.6) can be written in another form as:

$$\boxed{z^+\nabla\cdot(\mathbf{q}^+ + c^+\mathbf{q}^l) + z^-\nabla\cdot(\mathbf{q}^- + c^-\mathbf{q}^l) = 0.} \tag{2.3.8}$$

In (2.3.5), the presence of molar volume $\overline{V}^\beta$ shows a link between φ^β and φc^β. For the constitutive equations, our attempt is to introduce them not dependent on φ^β but on φc^β. As we will see later $\overline{V}^\beta$ will help us for this purpose.

Introducing the restriction equation (2.3.6) into inequality (2.3.3) by means of a Lagrange multiplier λ, yields:

$$\begin{aligned}
- & \frac{D^sW}{Dt} + J^s(\boldsymbol{\sigma} + p\boldsymbol{\mathcal{I}}) : \nabla\mathbf{v}^s + J^s(-\boldsymbol{\mathcal{K}}^l + p\varphi\boldsymbol{\mathcal{I}}) : \nabla(\mathbf{v}^l - \mathbf{v}^s) \\
+ & J^s \sum_{\beta=+,-} \left(-\boldsymbol{\mathcal{K}}^\beta + \frac{z^\beta\lambda}{\overline{V}^\beta}\varphi^\beta\boldsymbol{\mathcal{I}}\right) : \nabla(\mathbf{v}^\beta - \mathbf{v}^s) \\
+ & J^s(-\nabla\cdot\boldsymbol{\mathcal{K}}^l + p\nabla\varphi)\cdot(\mathbf{v}^l - \mathbf{v}^s) \\
+ & J^s \sum_{\beta=+,-} \left(-\nabla\cdot\boldsymbol{\mathcal{K}}^\beta + \frac{z^\beta\lambda}{\overline{V}^\beta}\nabla\varphi^\beta\right)\cdot(\mathbf{v}^\beta - \mathbf{v}^s) \geq 0.
\end{aligned} \tag{2.3.9}$$

To close the system, we choose W, $\boldsymbol{\sigma}+p\boldsymbol{\mathcal{I}}$, $-\boldsymbol{\mathcal{K}}^l+\varphi p\boldsymbol{\mathcal{I}}$, $-\boldsymbol{\mathcal{K}}^\beta+\frac{z^\beta\lambda}{\overline{V}^\beta}\varphi^\beta\boldsymbol{\mathcal{I}}$ $(\beta=+,-)$, $-\nabla\cdot\boldsymbol{\mathcal{K}}^l+p\nabla\varphi$ and $-\nabla\cdot\boldsymbol{\mathcal{K}}^\beta+\frac{z^\beta\lambda}{\overline{V}^\beta}\nabla\varphi^\beta$ $(\beta=+,-)$ to be the constitutive variables, i.e., they are functions of a set of independent variables (the constitutive variables are thus the dependent variables). We choose as independent variables the Green strain $\boldsymbol{\mathcal{E}}$ (cf. (2.1.5)), and the Lagrangian forms of the volume fractions of the liquid and the ions Φ^β, and the relative velocities $\mathbf{v}^{\beta s} = (\boldsymbol{\mathcal{F}}^s)^{-1}(\mathbf{v}^\beta - \mathbf{v}^s)$, $\beta = l,+,-$. Thus

$$W = W(\boldsymbol{\mathcal{E}}, \Phi^\beta, \mathbf{v}^{\beta s}), \tag{2.3.10}$$

$$\boldsymbol{\sigma} + p\boldsymbol{\mathcal{I}} = \frac{1}{J^s}\boldsymbol{\mathcal{F}}^s\widetilde{\boldsymbol{\mathcal{S}}}(\boldsymbol{\mathcal{E}}, \Phi^\beta, \mathbf{v}^{\beta s})(\boldsymbol{\mathcal{F}}^s)^T, \tag{2.3.11}$$

$$-\boldsymbol{\mathcal{K}}^l + p\varphi\boldsymbol{\mathcal{I}} = \boldsymbol{\mathcal{F}}^s\widetilde{\boldsymbol{\mathcal{K}}}^l(\boldsymbol{\mathcal{E}}, \Phi^\beta, \mathbf{v}^{\beta s})(\boldsymbol{\mathcal{F}}^s)^T, \tag{2.3.12}$$

$$-\boldsymbol{\mathcal{K}}^\beta + \frac{z^\beta\lambda}{\overline{V}^\beta}\varphi^\beta\boldsymbol{\mathcal{I}} = \boldsymbol{\mathcal{F}}^s\widetilde{\boldsymbol{\mathcal{K}}}^\beta(\boldsymbol{\mathcal{E}}, \Phi^\beta, \mathbf{v}^{\beta s})(\boldsymbol{\mathcal{F}}^s)^T,\ \beta = +,-, \tag{2.3.13}$$

$$-\nabla\cdot\boldsymbol{\mathcal{K}}^l + p\nabla\varphi = \boldsymbol{\mathcal{F}}^s\widetilde{\widetilde{\boldsymbol{\mathcal{K}}}}^l(\boldsymbol{\mathcal{E}}, \Phi^\beta, \mathbf{v}^{\beta s}), \tag{2.3.14}$$

$$-\nabla\cdot\boldsymbol{\mathcal{K}}^\beta + \frac{z^\beta\lambda}{\overline{V}^\beta}\nabla\varphi^\beta = \boldsymbol{\mathcal{F}}^s\widetilde{\widetilde{\boldsymbol{\mathcal{K}}}}^\beta(\boldsymbol{\mathcal{E}}, \Phi^\beta, \mathbf{v}^{\beta s}),\ \beta = +,-. \tag{2.3.15}$$

We apply the chain rule for the time differentiation of W, hence we have

$$\begin{aligned}\frac{D^sW}{Dt} &= \frac{\partial W}{\partial \boldsymbol{\mathcal{E}}} : \frac{D^s\boldsymbol{\mathcal{E}}}{Dt} + \sum_{\beta=l,+,-} \frac{\partial W}{\partial \Phi^\beta}\frac{D^s\Phi^\beta}{Dt} + \sum_{\beta=l,+,-} \frac{\partial W}{\partial \mathbf{v}^{\beta s}} \cdot \frac{D^s\mathbf{v}^{\beta s}}{Dt} \\ &= \boldsymbol{\mathcal{F}}^s \frac{\partial W}{\partial \boldsymbol{\mathcal{E}}} (\boldsymbol{\mathcal{F}}^s)^T : \nabla \mathbf{v}^s - J^s \sum_{\beta=l,+,-} \frac{\partial W}{\partial \Phi^\beta} \nabla \cdot \left(\varphi^\beta(\mathbf{v}^\beta - \mathbf{v}^s)\right) \\ &+ \sum_{\beta=l,+,-} \frac{\partial W}{\partial \mathbf{v}^{\beta s}} \cdot \frac{D^s\mathbf{v}^{\beta s}}{Dt}. \end{aligned} \tag{2.3.16}$$

Here we use that

$$\frac{D^s\boldsymbol{\mathcal{E}}}{Dt} = (\boldsymbol{\mathcal{F}}^s)^T \nabla \mathbf{v}^s \boldsymbol{\mathcal{F}}^s.$$

We insert the equation (2.3.16) in (2.3.9). This results into

$$\begin{aligned} &\left(J^s(\boldsymbol{\sigma} + p\boldsymbol{\mathcal{I}}) - \boldsymbol{\mathcal{F}}^s \frac{\partial W}{\partial \boldsymbol{\mathcal{E}}} (\boldsymbol{\mathcal{F}}^s)^T\right) : \nabla \mathbf{v}^s - \sum_{\beta=l,+,-} \frac{\partial W}{\partial \mathbf{v}^{\beta s}} \cdot \frac{D^s\mathbf{v}^{\beta s}}{Dt} \\ + \;& J^s \left(-\boldsymbol{\mathcal{K}}^l + \left(p + \frac{\partial W}{\partial \Phi}\right)\varphi \boldsymbol{\mathcal{I}}\right) : \nabla(\mathbf{v}^l - \mathbf{v}^s) \\ + \;& J^s \sum_{\beta=+,-} \left(-\boldsymbol{\mathcal{K}}^\beta + \left(\frac{z^\beta \lambda}{\overline{V}^\beta} + \frac{\partial W}{\partial \Phi^\beta}\right)\varphi^\beta \boldsymbol{\mathcal{I}}\right) : \nabla(\mathbf{v}^\beta - \mathbf{v}^s) \\ + \;& J^s \sum_{\beta=l,+,-} \mathbf{f}^\beta \cdot (\mathbf{v}^\beta - \mathbf{v}^s) \geq 0, \end{aligned}$$

where

$$\begin{aligned} \mathbf{f}^l &= -\nabla \cdot \boldsymbol{\mathcal{K}}^l + \left(p + \frac{\partial W}{\partial \Phi}\right)\nabla\varphi, \\ \mathbf{f}^\beta &= -\nabla \cdot \boldsymbol{\mathcal{K}}^\beta + \left(\frac{z^\beta \lambda}{\overline{V}^\beta} + \frac{\partial W}{\partial \Phi^\beta}\right)\nabla\varphi^\beta, \quad \beta = +,-. \end{aligned}$$

It follows from (2.3.10), (2.3.14) and (2.3.15) that

$$\mathbf{f}^\beta = \boldsymbol{\mathcal{F}}^s \tilde{\mathbf{f}}^\beta(\boldsymbol{\mathcal{E}}, \Phi^\beta, \mathbf{v}^{\beta s}), \quad \beta = l,+,-. \tag{2.3.17}$$

By a standard argument (Coleman and Noll, 1963), (2.3.17) is satisfied if and only if

$$\boldsymbol{\sigma} + p\boldsymbol{\mathcal{I}} = \frac{1}{J^s}\boldsymbol{\mathcal{F}}^s \frac{\partial W}{\partial \boldsymbol{\mathcal{E}}}(\boldsymbol{\mathcal{F}}^s)^T, \tag{2.3.18}$$

$$\frac{\partial W}{\partial \mathbf{v}^{\beta s}} = 0, \quad \beta = l, +, -, \tag{2.3.19}$$

$$\boldsymbol{\mathcal{K}}^l = \left(p + \frac{\partial W}{\partial \Phi}\right)\varphi\boldsymbol{\mathcal{I}}, \tag{2.3.20}$$

$$\boldsymbol{\mathcal{K}}^\beta = \left(\frac{z^\beta \lambda}{\overline{V}^\beta} + \frac{\partial W}{\partial \Phi^\beta}\right)\varphi^\beta \boldsymbol{\mathcal{I}}, \quad \beta = +, -, \tag{2.3.21}$$

and

$$\sum_{\beta=l,+,-} \mathbf{f}^\beta \cdot (\mathbf{v}^\beta - \mathbf{v}^s) \geq 0. \tag{2.3.22}$$

Equation (2.3.18) shows that the stress of the mixture can be derived from the strain energy function W minus $p\boldsymbol{\mathcal{I}}$. It can be seen that here p presents the hydrostatic pressure acting on the mixture (Bowen, 1980). Equation (2.3.19) shows that the strain energy does not depend on the relative velocities. Define the chemical potential μ^l per unit fluid volume and the electro-chemical potential μ^β, $\beta = +, -$, per mol of ion β, such that

$$\boldsymbol{\mathcal{K}}^l = \varphi\mu^l\boldsymbol{\mathcal{I}}, \tag{2.3.23}$$

$$\boldsymbol{\mathcal{K}}^\beta = \varphi c^\beta \mu^\beta \boldsymbol{\mathcal{I}}, \quad \beta = +, -. \tag{2.3.24}$$

Therefore equations (2.3.20) and (2.3.21) imply that

$$\boxed{\begin{aligned} \mu^l &= p + \frac{\partial W}{\partial \Phi}, \\ \mu^\beta &= \lambda z^\beta + \frac{\partial W}{\partial \Phi^\beta}\overline{V}^\beta, \quad \beta = +, -. \end{aligned}} \tag{2.3.25}$$

It has been shown (Huyghe and Janssen, 1997) that the multiplier λ can be interpreted as the electrical potential of the medium multiplied by the constant of Faraday, i.e., $\lambda = F\xi$.

We use the residual inequality (2.3.22) to establish

$$\tilde{\mathbf{f}}^\beta(\boldsymbol{\mathcal{E}}, \Phi^\beta, \mathbf{0}) = \mathbf{0}, \quad \beta = l, +, -. \tag{2.3.26}$$

It is natural to refer to the state where $\mathbf{v}^{ls} = \mathbf{v}^{+s} = \mathbf{v}^{-s} = \mathbf{0}$ as the state of thermodynamic equilibrium. Equation (2.3.26) shows that local interaction forces vanish in this state. In the approximation where the departures from the state $\nabla_0\Phi^\beta = \mathbf{0}$ (∇_0 is the gradient in initial configuration) and $\mathbf{v}^{\beta s} = \mathbf{0}$, for $\beta = l, +, -$, are assumed to be small, (2.3.17) can be approximated by

$$\mathbf{f}^\beta = \sum_{\gamma=l,+,-} B^{\beta\gamma}(\mathbf{v}^\gamma - \mathbf{v}^s), \quad \beta = l, +, -, \tag{2.3.27}$$

where

$$B^{\beta\gamma} = \boldsymbol{\mathcal{F}}^s \frac{\partial \tilde{\mathbf{f}}^\beta}{\partial \mathbf{v}^{\gamma s}}(\boldsymbol{\mathcal{E}}, \Phi^\gamma, \mathbf{0})(\boldsymbol{\mathcal{F}}^s)^T, \quad \beta, \gamma = l, +, -. \tag{2.3.28}$$

Given (2.3.22) and (2.3.27), we can conclude that $\mathbf{B}$ is a positive symmetric semi-definite matrix.

Substituting (2.3.25) into equation (2.3.27) and using the approximation of $\mathbf{f}^\beta$ we get the classical equations of irreversible thermodynamics:

$$\begin{cases} -\varphi^l \nabla \mu^l & = \sum_{\gamma=l,+,-} B^{l\gamma}(\mathbf{v}^\gamma - \mathbf{v}^s), \\ -\dfrac{\varphi^\beta}{\overline{V}^\beta} \nabla \mu^\beta & = \sum_{\gamma=l,+,-} B^{\beta\gamma}(\mathbf{v}^\gamma - \mathbf{v}^s), \quad \beta = +, -. \end{cases} \tag{2.3.29}$$

As it is assumed in the previous section, we restrict our considerations to isothermal, non-reacting mixtures where the solid phase is homogeneous. For such a mixture that consists of four-component, the Helmholtz potential is expressed as a sum of an elastic energy $W_E(\boldsymbol{\mathcal{E}})$ and a mixing energy $W(\Phi^\beta)$ for $\beta = l, +, -$, Huyghe and Janssen (1997). Define

$$\begin{aligned} W(\boldsymbol{\mathcal{E}}, \Phi, \Phi^+, \Phi^-) &= (\mu_0^l + RTc)\Phi + \mu_0^+ \frac{\Phi^+}{\overline{V}^+} + \mu_0^- \frac{\Phi^-}{\overline{V}^-} \\ &+ RT(\Phi c - \frac{\Phi^+}{\overline{V}^+} - \frac{\Phi^-}{\overline{V}^-}) \left(\ln \frac{\Phi c - \dfrac{\Phi^+}{\overline{V}^+} - \dfrac{\Phi^-}{\overline{V}^-}}{\Phi c} - 1 \right) \\ &+ RT\Gamma^+ \frac{\Phi^+}{\overline{V}^+} \left(\ln \frac{\Phi^+}{\Phi c \overline{V}^+} - 1 \right) \\ &+ RT\Gamma^- \frac{\Phi^-}{\overline{V}^-} \left(\ln \frac{\Phi^-}{\Phi c \overline{V}^-} - 1 \right) + W_E(\boldsymbol{\mathcal{E}}). \end{aligned} \tag{2.3.30}$$

In this relation:

- μ_0^l is the initial electro-chemical potential of the fluid phase,
- μ_0^β is the initial electro-chemical potential of ion β,
- $\Gamma^\beta \in (0, 1]$ is the osmotic coefficient of ion β, which is uniform and constant,
- c is the molar concentration of the fluid phase, which is assumed to be uniform and constant,
- R is the universal gas constant,
- T is the absolute temperature, which is uniform and constant since the materials are assumed to be isothermal.

The constitutive equations (2.3.18) and (2.3.29) that fulfil the second law of thermodynamics are

$$\boldsymbol{\sigma} + p\boldsymbol{\mathcal{I}} = \frac{1}{J^s}\boldsymbol{\mathcal{F}}^s \frac{\partial W}{\partial \boldsymbol{\mathcal{E}}}(\boldsymbol{\mathcal{F}}^s)^T, \tag{2.3.31}$$

$$-\varphi^\beta \nabla \tilde{\mu}^\beta = \sum_{\gamma=l,+,-} B^{\beta\gamma}(\mathbf{v}^\gamma - \mathbf{v}^s), \quad \beta = l,+,-, \tag{2.3.32}$$

with $\tilde{\mu}^l = \mu^l$, $\tilde{\mu}^\beta = \mu^\beta/\overline{V}^\beta$, $(\beta = +,-)$.

By using equations (2.3.25) and (2.3.30) we simplify the equations for the electrochemical potentials

$$\begin{aligned} \mu^l = p + \frac{\partial W}{\partial \Phi} &= p + \mu_0^l + RTc \ln \frac{\Phi c - \dfrac{\Phi^+}{\overline{V}^+} - \dfrac{\Phi^-}{\overline{V}^-}}{\Phi c} \\ &+ \frac{RT}{\Phi}\left(\frac{\Phi^+}{\overline{V}^+} + \frac{\Phi^-}{\overline{V}^-}\right) \\ &- \frac{RT\Gamma^+\Phi^+}{\overline{V}^+\Phi} - \frac{RT\Gamma^-\Phi^-}{\overline{V}^-\Phi}, \end{aligned} \tag{2.3.33}$$

and

$$\begin{aligned} \mu^\beta = z^\beta F\xi + \frac{\partial W}{\partial \Phi^\beta}\overline{V}^\beta &= z^\beta F\xi + \mu_0^\beta - RT \ln \frac{\Phi c - \dfrac{\Phi^+}{\overline{V}^+} - \dfrac{\Phi^-}{\overline{V}^-}}{\Phi c} \\ &+ RT\Gamma^\beta \ln \frac{\Phi^\beta}{\Phi c \overline{V}^\beta}, \quad \beta = +,-. \end{aligned} \tag{2.3.34}$$

After linearising the logarithm terms and using (2.3.7) we have

$$\boxed{\begin{aligned} \mu^l &\approx p + \mu_0^l - RT(\Gamma^+ c^+ + \Gamma^- c^-) \\ \mu^\beta &\approx \mu_0^\beta + z^\beta F\xi + RT\Gamma^\beta \ln \frac{c^\beta}{c}, \quad \beta = +,-. \end{aligned}} \tag{2.3.35}$$

In (Molenaar et .al, 1999) the components of the friction matrix are related to diffusion coefficients of fluid and ions and it can be shown that

$$B^{ll} = \varphi^2 K^{-1} - (B^{l+} + B^{l-}), \tag{2.3.36}$$

$$B^{ii} = -B^{il}, \quad i = +,-, \tag{2.3.37}$$

$$B^{il} = -\varphi^i RT(\overline{V}^i D^i)^{-1}, \quad i = +,-, \tag{2.3.38}$$

$$B^{+-} = 0, \tag{2.3.39}$$

where K is the permeability and D^i is the ion diffusion tensor in free water. Manipulation of the second equation in (2.3.32) yields

$$\boxed{\varphi^\beta(\mathbf{v}^\beta - \mathbf{v}^s) = -\sum_{\gamma=l,+,-} P^{\beta\gamma}\nabla\tilde{\mu}^\gamma, \quad \beta = l,+,-,} \tag{2.3.40}$$

with

$$P^{\beta\gamma} = \varphi^\beta\varphi^\gamma(B^{-1})^{\beta\gamma}, \quad \beta,\gamma = l,+,-.$$

$\mathbf{P} = (P^{\beta\gamma})_{\beta,\gamma=l,+,-}$ can be derived as:

$$\mathbf{P} = \begin{pmatrix} K & K\dfrac{\varphi^+}{\varphi} & K\dfrac{\varphi^-}{\varphi} \\ K\dfrac{\varphi^+}{\varphi} & \dfrac{\overline{V}^+D^+\varphi^+}{RT} + K\left(\dfrac{\varphi^+}{\varphi}\right)^2 & K\dfrac{\varphi^+\varphi^-}{\varphi^2} \\ K\dfrac{\varphi^-}{\varphi} & K\dfrac{\varphi^+\varphi^-}{\varphi^2} & \dfrac{\overline{V}^-D^-\varphi^-}{RT} + K\left(\dfrac{\varphi^-}{\varphi}\right)^2 \end{pmatrix}. \tag{2.3.41}$$

Now by using (2.3.40) we can derive the specific discharge $\mathbf{q}^l$ and the ion fluxes $\mathbf{q}^i$ in terms of the electro-chemical potential μ^β,

$$\begin{aligned} \mathbf{q}^l = \varphi(\mathbf{v}^l - \mathbf{v}^s) &= -\sum_{\gamma=l,+,-} P^{l\gamma}\nabla\tilde{\mu}^\gamma \\ &= -\frac{K}{\varphi}(\nabla\tilde{\mu}^l + \varphi^+\nabla\tilde{\mu}^+ + \varphi^-\nabla\tilde{\mu}^-) \\ &= -K(\nabla\mu^l + c^+\nabla\mu^+ + c^-\nabla\mu^-), \end{aligned} \tag{2.3.42}$$

and

$$\begin{aligned} \mathbf{q}^\beta = \frac{\varphi^\beta}{\overline{V}^\beta}(\mathbf{v}^\beta - \mathbf{v}^l) &= \frac{\varphi^\beta}{\overline{V}^\beta}(\mathbf{v}^\beta - \mathbf{v}^s) - \frac{\varphi^\beta}{\overline{V}^\beta}(\mathbf{v}^l - \mathbf{v}^s) \\ &= -\frac{1}{\overline{V}^\beta}\sum_{\gamma=l,+,-} P^{\beta\gamma}\nabla\tilde{\mu}^\gamma - c^\beta\mathbf{q}^l \\ &= -\frac{D^\beta c^\beta\varphi}{RT}\nabla\mu^\beta, \quad \beta = +,-. \end{aligned} \tag{2.3.43}$$

The above relations are called the extended Darcy's law and Fick's law.

Assuming the electro-neutrality (2.2.11), if we put (2.3.35) into (2.3.42) and (2.3.43), then the extended Darcy's law and the Fick's law can be stated in terms of the variables p, c^β and ξ as follow:

$$\boxed{\begin{aligned} \mathbf{q}^l &= -K\left(\nabla p - z^{fc}c^{fc}F\nabla\xi\right), \\ \mathbf{q}^\beta &= -D^\beta\varphi\left(\frac{F}{RT}z^\beta c^\beta\nabla\xi + \Gamma^\beta\nabla c^\beta\right), \quad \beta = +,-. \end{aligned}} \tag{2.3.44}$$

From physical considerations (Huyghe and Janssen, 1997), μ^l and μ^β are continuous even if c^{fc} is not. Therefore we choose the electro-chemical potentials to be the primal variables.

Remark 2.5. *Define the activity f^β by*

$$f^\beta = \left(\frac{c^\beta}{c}\right)^{\Gamma^\beta - 1}, \quad \beta = +, -. \tag{2.3.45}$$

Then based on the definition of the electro-chemical potentials and on the electro-neutrality assumption, the secondary variables c^β, p and ξ are expressed as

$$c^\beta = -\frac{1}{2z^\beta} z^{fc} c^{fc} + \frac{1}{2}\sqrt{(z^{fc}c^{fc})^2 + \frac{4c^2}{f^+ f^-}\exp\frac{\mu^+ - \mu_0^+ + \mu^- - \mu_0^-}{RT}}, \tag{2.3.46}$$

$$p = \mu^l - \mu_0^l + RT\left(\Gamma^+ c^+ + \Gamma^- c^-\right), \tag{2.3.47}$$

$$\xi = \frac{1}{z^\beta F}\left(\mu^\beta - \mu_0^\beta - RT\ln\frac{f^\beta c^\beta}{c}\right), \quad \beta = +, -. \tag{2.3.48}$$

The ion concentrations c^β are clearly positive. For numerical stability, it is preferable to use the expression for voltage with $\beta = -$ if z^{fc} is positive and vice versa.

2.4 Reformulation in Lagrangian coordinates

From now, we omit the superscript 's' from $\boldsymbol{\mathcal{F}}^s$ and J^s and $\frac{D^s}{Dt}$. For a scalar a, a vector $\mathbf{a}$ and a tensor $\boldsymbol{\mathcal{T}}$, the following relations hold for gradient and divergence operators in the reference configuration and the current configuration (Chadwick, 1999, page 59).

$$\begin{aligned}
\boldsymbol{\mathcal{F}}^{-T}\nabla_0 a &= \nabla a, \\
\frac{1}{J}\nabla_0 \cdot (J\boldsymbol{\mathcal{F}}^{-1}\mathbf{a}) &= \nabla \cdot \mathbf{a}, \\
\frac{1}{J}\nabla_0 \cdot (J\boldsymbol{\mathcal{F}}^{-1}\boldsymbol{\mathcal{T}}) &= \nabla \cdot \boldsymbol{\mathcal{T}}.
\end{aligned}$$

Define the displacement field in Lagrangian and Eulerian form by

$$\begin{aligned}
\mathbf{U}(\mathbf{X}, t) &= \mathbf{x}(\mathbf{X}, t) - \mathbf{X}, \\
\mathbf{u}(\mathbf{x}, t) &= \mathbf{x} - \mathbf{X}(\mathbf{x}, t),
\end{aligned}$$

respectively.

Let us choose the configuration $\Omega_{t_0} \subset \mathbb{R}^3$ of the solid skeleton at the initial instant of time t_0 as the reference configuration for the Lagrangian description. The

reference configuration need not to be a stress-free configuration. In fact, the stress $\mathbf{\Pi}_0$ is defined in the reference configuration and obeys the momentum balance

$$\nabla_0 \cdot \mathbf{\Pi}_0 = \mathbf{0}.$$

Define φ_0 and $\varphi_0^s = 1 - \varphi_0$ as the initial porosity and the initial volume fraction of the solid phase, respectively. Recall the Lagrangian form of the balance equation in (2.3.2):

$$\frac{DJ\varphi^\alpha}{Dt} + J\nabla \cdot (\varphi^\alpha(\mathbf{v}^\alpha - \mathbf{v}^s)) = 0, \quad \alpha = s, l, +, -.$$

It can be easily seen that the above equation is equivalent to

$$\frac{DJ\varphi^\alpha}{Dt} + \nabla_0 \cdot \left(J\boldsymbol{\mathcal{F}}^{-1}\varphi^\alpha(\mathbf{v}^\alpha - \mathbf{v}^s)\right) = 0, \quad \alpha = s, l, +, -.$$

For $\alpha = s$ we have

$$\frac{DJ\varphi^s}{Dt} = 0, \quad \text{or} \quad \varphi^s J = \varphi_0^s.$$

where φ_0^s is the solid volume fraction in the reference configuration. This gives

$$\boxed{\varphi = 1 - \varphi^s = 1 - \frac{1 - \varphi_0}{J}.} \tag{2.4.1}$$

For $\alpha = l$ we obtain

$$\boxed{\frac{DJ\varphi}{Dt} + \nabla_0 \cdot \mathfrak{Q}^l = 0,} \tag{2.4.2}$$

where

$$\mathfrak{Q}^l = J\boldsymbol{\mathcal{F}}^{-1}\mathbf{q}^l. \tag{2.4.3}$$

By using definitions (2.2.5), (2.2.7) and equation (2.3.2), we have

$$\frac{DJ\varphi c^\beta}{Dt} + J\nabla \cdot (\mathbf{q}^\beta + c^\beta \mathbf{q}^l) = 0, \quad \beta = +, -.$$

The ions balance in Lagrangian form takes the following form

$$\boxed{\frac{DJ\varphi c^\beta}{Dt} + \nabla_0 \cdot (\mathfrak{Q}^\beta + c^\beta \mathfrak{Q}^l) = 0, \quad \beta = +, -,} \tag{2.4.4}$$

where

$$\mathfrak{Q}^\beta = J\boldsymbol{\mathcal{F}}^{-1}\mathbf{q}^\beta, \quad \beta = +, -. \tag{2.4.5}$$

In the Lagrangian form, (2.2.12) is expressed as

$$\frac{DJ\varphi c^{fc}}{Dt} = 0, \quad \text{or} \quad \varphi c^{fc} = \varphi_0 c_0^{fc} J^{-1}, \tag{2.4.6}$$

where c_0^{fc} is the fixed charge concentration in the reference configuration. From (2.4.1) follows,

$$(\varphi J)^{-1} = (J - \varphi_0^s)^{-1},$$

therefore

$$\boxed{c^{fc} = c_0^{fc}\varphi_0(J - \varphi_0^s)^{-1}.} \tag{2.4.7}$$

Define the first and second Piola-Kirchhoff stress tensors by

$$\begin{aligned} \boldsymbol{\Pi} &= J\boldsymbol{\sigma}\boldsymbol{\mathcal{F}}^{-T}, \\ \boldsymbol{\mathcal{S}} &= J\boldsymbol{\mathcal{F}}^{-1}\boldsymbol{\sigma}\boldsymbol{\mathcal{F}}^{-T}, \end{aligned}$$

respectively. Then equation (2.2.10) in Lagrangian form takes the following form

$$\boxed{\nabla_0 \cdot \boldsymbol{\Pi} = \mathbf{0} \quad \text{or} \quad \nabla_0 \cdot \left(\boldsymbol{\mathcal{S}}\boldsymbol{\mathcal{F}}^T\right) = \mathbf{0},} \tag{2.4.8}$$

The constitutive relation (2.3.31) is given by

$$\boldsymbol{\sigma} + p\boldsymbol{\mathcal{I}} = \frac{1}{J}\boldsymbol{\mathcal{F}}\frac{\partial W}{\partial \boldsymbol{\mathcal{E}}}\boldsymbol{\mathcal{F}}^T,$$

Considering this relation, the second Piola-Kirchhoff stress is expressed by

$$\boxed{\boldsymbol{\mathcal{S}} = \boldsymbol{\Pi}\boldsymbol{\mathcal{F}}^{-T} = \frac{\partial W}{\partial \boldsymbol{\mathcal{E}}} - pJ\boldsymbol{\mathcal{C}}^{-1},} \tag{2.4.9}$$

where the right Cauchy-Green tensor $\boldsymbol{\mathcal{C}}$ is defined in (2.1.4).

It is easy to check that the Lagrangian form of equations (2.3.42) and (2.3.43) is

$$\boxed{\begin{aligned} \mathfrak{G}^l &= -\widetilde{\boldsymbol{\mathcal{K}}}(\nabla_0\mu^l + c^+\nabla_0\mu^+ + c^-\nabla_0\mu^-), \\ \mathfrak{G}^\beta &= -\frac{\widetilde{\boldsymbol{\mathcal{D}}}^\beta c^\beta\varphi}{RT}\nabla_0\mu^\beta, \quad \beta = +,-, \end{aligned}} \tag{2.4.10}$$

where

$$\widetilde{\boldsymbol{\mathcal{K}}} = J\boldsymbol{\mathcal{F}}^{-1}K\boldsymbol{\mathcal{F}}^{-T}, \tag{2.4.11}$$

$$\widetilde{\boldsymbol{\mathcal{D}}}^\beta = J\boldsymbol{\mathcal{F}}^{-1}D^\beta\boldsymbol{\mathcal{F}}^{-T}, \quad \beta = +,-. \tag{2.4.12}$$

2.5 Total set of equations

The combination of the deformation of the porous media and the flow of the fluid and ions in the Lagrangian description results into the following set of equations:

Balance Equations

$$\begin{aligned} \nabla_0 \cdot (\boldsymbol{\mathcal{S}}\boldsymbol{\mathcal{F}}^T) &= \mathbf{0}, \\ \frac{DJ\varphi}{Dt} + \nabla_0 \cdot \mathfrak{Q}^l &= 0, \\ \frac{DJ\varphi c^\beta}{Dt} + \nabla_0 \cdot (\mathfrak{Q}^\beta + c^\beta \mathfrak{Q}^l) &= 0, \quad \beta = +, -, \end{aligned} \tag{2.5.1}$$

Constitutive Equations

$$\begin{aligned} \frac{\partial W}{\partial \boldsymbol{\mathcal{E}}} - pJ\boldsymbol{\mathcal{C}}^{-1} &= \boldsymbol{\mathcal{S}}, \\ -\widetilde{\boldsymbol{\mathcal{K}}}(\nabla_0 \mu^l + c^+ \nabla_0 \mu^+ + c^- \nabla_0 \mu^-) &= \mathfrak{Q}^l, \\ -\frac{\widetilde{\boldsymbol{\mathcal{D}}}^\beta c^\beta \varphi}{RT} \nabla_0 \mu^\beta &= \mathfrak{Q}^\beta, \quad \beta = +, -. \end{aligned}$$

2.6 Donnan equilibrium and boundary conditions

In order to solve the above system of equations, we need to pose the boundary conditions. This can be achieved by suitably combining the essential conditions for μ^l, μ^β and $\mathbf{U}$ and the natural conditions for the normal components of $\mathfrak{Q}^\beta$, $\beta = l, +, -$, and $\boldsymbol{\mathcal{S}}$.
Consider the case that the porous medium is in contact with an electro-neutral bathing solution, given that the pressure p_{out}, the voltage ξ_{out} and the ion concentrations c_{out} are known. The bathing solution contains no fixed charges, thus $c^+_{out} = c^-_{out} = c_{out}$. Since the electro-chemical potentials are continuous at the boundary,

$$\mu^l_{in} = \mu^l_{out}, \tag{2.6.1}$$
$$\mu^+_{in} = \mu^+_{out}, \tag{2.6.2}$$
$$\mu^-_{in} = \mu^-_{out}, \tag{2.6.3}$$

where μ^l_{out} and μ^β_{out} are the electro-chemical potentials in the outer solution. Assume $\Gamma^+_{in} = \Gamma^-_{in} = \Gamma$ and $\Gamma^+_{out} = \Gamma^-_{out} = 1$, then the combination of the above relations and the relations expressed in (2.3.35) provide

$$\mu^l_{in} = \mu^l_0 + p_{out} - 2RTc_{out}, \tag{2.6.4}$$
$$\mu^\beta_{in} = \mu^\beta_0 + Fz^\beta \xi_{out} + RT \ln \frac{c_{out}}{c}, \quad \beta = +, -, \tag{2.6.5}$$

where, c_{out}, p_{out} and ξ_{out} are the ions concentration, fluid pressure and the electrical potential of the outer solution, respectively. Equation (2.6.5) for $\beta = +, -$ in

combination with (2.6.2) and (2.6.3) imply

$$\mu_0^+ + \mu_0^- + RT \ln \frac{c_{out}^2}{c^2} = \mu_{out}^+ + \mu_{out}^- = \mu_{in}^+ + \mu_{in}^- = \mu_0^+ + \mu_0^- + RT\Gamma \ln \frac{c_{in}^+ c_{in}^-}{c^2},$$

Therefore, we have

$$\frac{c_{out}^2}{c^2} = \left(\frac{c_{in}^+ c_{in}^-}{c^2} \right)^{\Gamma}. \tag{2.6.6}$$

Easily we can see that

$$\pi = p_{in} - p_{out} = RT \left(\Gamma(c_{in}^+ + c_{in}^-) - 2c_{out} \right), \tag{2.6.7}$$

$$\xi_{in} - \xi_{out} = \frac{RT}{Fz^\beta} \ln \frac{c_{out} c^{\Gamma-1}}{(c_{in}^\beta)^\Gamma}, \quad \beta = +, -, \tag{2.6.8}$$

In the above relations, π is the osmotic pressure (Richards, 1980) and $\xi_{in} - \xi_{out}$ is the Donnan voltage between the inner and outer solution. It is also called the Nernst potential (Gu et al., 1999), (Helfferich, 1962).

Let Ω be an open domain in $\mathbb{R}^n$, $n = 1, 2, 3$, then define $\Omega_T = \Omega \times (0, T]$ for $T > 0$ and consider the sets $\Gamma_{\mathbf{u}}^D$ and $\Gamma_{\mathbf{u}}^N$ (and similarly Γ_p^D and Γ_p^N) to be two disjoint open subsets of the total boundary $\Gamma = \partial\Omega$, such that $\Gamma_\alpha^D \cap \Gamma_\alpha^N = \emptyset$ and $\bar{\Gamma}_\alpha^D \cup \bar{\Gamma}_\alpha^N = \Gamma$ for $\alpha = \mathbf{u}$ and p. We assume

$$\text{meas } \Gamma_\alpha^D > 0 \quad \text{for } \alpha = \mathbf{u}, p. \tag{2.6.9}$$

From the above statements we can get the following boundary conditions:

Boundary Conditions

$$\begin{aligned}
\mathbf{U} &= \mathbf{0} && \text{on } \Gamma_{\mathbf{u}}^D \times (0,T], \\
\mu^l &= \mu_{in}^l && \text{on } \Gamma_p^D \times (0,T], \\
\mu^+ &= \mu_{in}^+ && \text{on } \Gamma_p^D \times (0,T], \\
\mu^- &= \mu_{in}^- && \text{on } \Gamma_p^D \times (0,T], \\
\mathbf{n} \cdot (\boldsymbol{\mathcal{S}}\boldsymbol{\mathcal{F}}^T) &= \mathbf{g}_{\mathbf{u}}^N && \text{on } \Gamma_{\mathbf{u}}^N \times (0,T], \\
\mathbf{n} \cdot \mathfrak{Q}^l &= 0 && \text{on } \Gamma_p^N \times (0,T], \\
\mathbf{n} \cdot \mathfrak{Q}^+ &= 0 && \text{on } \Gamma_p^N \times (0,T], \\
\mathbf{n} \cdot \mathfrak{Q}^- &= 0 && \text{on } \Gamma_p^N \times (0,T].
\end{aligned} \tag{2.6.10}$$

2.7 Reduction to infinitesimal deformation

In this section we keep all the assumption from the previous sections, but we also assume infinitesimal deformation for the solid phase.

In the infinitesimal theory of elasticity it is assumed that the components of the displacement vector and their spatial derivatives are infinitesimal of the first order so

that we neglect products and squares of these quantities in comparison with their first powers (Fluügge, 1958, page 6). Using this approximation we find the deformation tensor and the strain tensor as

$$\boldsymbol{\mathcal{F}} = \boldsymbol{\mathcal{I}} + \nabla_0 \mathbf{U}, \quad \boldsymbol{\mathcal{E}} = \frac{1}{2}(\nabla_0 \mathbf{U} + (\nabla_0 \mathbf{U})^T), \tag{2.7.1}$$

where $\mathbf{U} = \mathbf{x} - \mathbf{X}$ is the displacement vector. Recall equation (2.4.1), since the solid phase is assumed to have infinitesimal deformation, the Taylor linearisation for J^{-1} at $\boldsymbol{\mathcal{F}} = \mathbf{I}$ implies

$$J^{-1} \approx 1 - \left(\frac{1}{J^2}\frac{\partial J}{\partial \boldsymbol{\mathcal{F}}}\right)\Bigg|_{\boldsymbol{\mathcal{F}}=\boldsymbol{\mathcal{I}}} : (\boldsymbol{\mathcal{F}} - \boldsymbol{\mathcal{I}}) = 1 - \nabla_0 \cdot \mathbf{U}.$$

In the above relation, we use the relation (Holzapfel, 2000, page 41)

$$\frac{\partial J}{\partial \boldsymbol{\mathcal{F}}} = J\boldsymbol{\mathcal{F}}^{-T}. \tag{2.7.2}$$

Putting the linearised form of J^{-1} into (2.4.1) results into

$$\boxed{\varphi = 1 - (1 - \varphi_0)(1 - \nabla_0 \cdot \mathbf{U}).} \tag{2.7.3}$$

Also remember the relation for fixed charges density in (2.4.7) given by

$$c^{fc} = c_0^{fc}\varphi_0(J - \varphi_0^s)^{-1}.$$

From the assumption of infinitesimal elastic deformation for the solid phase, the Taylor linearisation for the function $(J - \varphi_0^s)^{-1}$ at $\boldsymbol{\mathcal{F}} = \boldsymbol{\mathcal{I}}$ results into

$$\begin{aligned}(J - \varphi_0^s)^{-1} &\approx (1 - \varphi_0^s)^{-1} - \left(\frac{1}{(J - \varphi_0^s)^2}\frac{\partial J}{\partial \boldsymbol{\mathcal{F}}}\right)\Bigg|_{\boldsymbol{\mathcal{F}}=\mathbf{I}} : (\boldsymbol{\mathcal{F}} - \boldsymbol{\mathcal{I}}) \\ &= \frac{1}{\varphi_0} - \frac{\nabla_0 \cdot \mathbf{U}}{\varphi_0^2}.\end{aligned} \tag{2.7.4}$$

Hence

$$\boxed{c^{fc} = c_0^{fc}\left(1 - \frac{\nabla_0 \cdot \mathbf{U}}{\varphi_0}\right).} \tag{2.7.5}$$

We choose a linear elastic material and therefore the elastic energy part is of the form

$$W_E(\boldsymbol{\mathcal{E}}) = \mu_s \boldsymbol{\mathcal{E}} : \boldsymbol{\mathcal{E}} + \frac{\lambda_s}{2}(\nabla_0 \cdot \mathbf{U})^2, \tag{2.7.6}$$

where λ_s and μ_s are the Lamé stress constants.

In the next step we will rewrite the equations in the infinitesimal deformation regime. Starting from the force balance and the related constitutive equation (2.4.9) we have

$$\begin{aligned} & \nabla_0 \cdot \left(\frac{\partial W}{\partial \boldsymbol{\mathcal{E}}} \boldsymbol{\mathcal{F}}^T \right) - \nabla_0 \cdot (pJ\boldsymbol{\mathcal{F}}^{-1}) = \mathbf{0}, \\ \text{or} \quad & \nabla_0 \cdot \left(\frac{\partial W}{\partial \boldsymbol{\mathcal{E}}} \boldsymbol{\mathcal{F}}^T \right) - J\nabla p = \mathbf{0}, \\ \text{or} \quad & \nabla_0 \cdot \left(\frac{\partial W}{\partial \boldsymbol{\mathcal{E}}} \boldsymbol{\mathcal{F}}^T \right) - J\boldsymbol{\mathcal{F}}^{-T}\nabla_0 p = \mathbf{0}, \end{aligned}$$

By using (2.7.1) the last equation is reduced to

$$\begin{aligned} & \nabla_0 \cdot (2\mu_s \boldsymbol{\mathcal{E}} + \lambda_s \nabla_0 \mathbf{U}) - \nabla_0 p + \nabla_0 \cdot \left((2\mu_s \boldsymbol{\mathcal{E}} + \lambda_s \nabla_0 \mathbf{U}) \nabla_0 \mathbf{U}^T \right) \\ + \quad & \nabla_0 \mathbf{U}^T \nabla_0 p - \nabla_0 \cdot \mathbf{U} \nabla_0 p + \nabla_0 \cdot \mathbf{U} \nabla_0 \mathbf{U}^T \nabla_0 p = \mathbf{0}. \end{aligned}$$

Assuming infinitesimal deformation for the solid phase, all terms except the first and second terms vanish and finally we have

$$\nabla_0 \cdot (2\mu_s \boldsymbol{\mathcal{E}} + \lambda_s \nabla_0 \cdot \mathbf{U}) - \nabla_0 p = \mathbf{0}.$$

Note that from (2.7.3), we have

$$J\varphi = (1 + \nabla_0 \cdot \mathbf{U}) \left(1 - (1 - \varphi_0)(1 - \nabla_0 \cdot \mathbf{U})\right) = \nabla_0 \cdot \mathbf{U} + \varphi_0.$$

The permeability $\widetilde{\boldsymbol{\mathcal{K}}}$ and diffusion tensors $\widetilde{\boldsymbol{\mathcal{D}}}^{\beta}$ are considered to be isotropic tensors represented by scalar multiple of the identity. To make the notations simpler, we change notations according to the following table:

Old notations	∇_0	D/Dt	$\mathfrak{q}^{\beta}$, $\beta = l, +, -$	$\mathbf{U}$	$\widetilde{\boldsymbol{\mathcal{D}}}^{\beta}$, $\beta = +, -$	$\widetilde{\boldsymbol{\mathcal{K}}}$
New notations	∇	$\partial/\partial t$	$\mathbf{q}^{\beta}$, $\beta = l, +, -$	$\mathbf{u}$	D^{β}, $\beta = +, -$	K

Table 2.1. New notations for infinitesimal deformation

Now the total set of equations is given by:

$$
\begin{array}{rcll}
\multicolumn{4}{l}{\textbf{Conservation Equations}} \\
\hline
\mathbf{0} &=& \nabla\cdot\boldsymbol{\sigma} - \nabla p, & \\
0 &=& \dfrac{\partial \nabla\cdot\mathbf{u}}{\partial t} + \nabla\cdot\mathbf{q}^l, & \\
0 &=& \dfrac{\partial(\nabla\cdot\mathbf{u}+\varphi_0)c^\beta}{\partial t} + \nabla\cdot(\mathbf{q}^\beta + c^\beta\mathbf{q}^l), & \beta = +,-, \\
\multicolumn{4}{l}{\textbf{Constitutive Equations}} \\
\hline
\boldsymbol{\sigma} &=& 2\mu_s\boldsymbol{\mathcal{E}} + \lambda_s \mathrm{tr}\boldsymbol{\mathcal{E}}, \quad \boldsymbol{\mathcal{E}} = \dfrac{1}{2}(\nabla\mathbf{u} + (\nabla\mathbf{u}^T)), & \\
\mathbf{q}^l &=& -K(\nabla\mu^l + c^+\nabla\mu^+ + c^-\nabla\mu^-), & \\
\mathbf{q}^\beta &=& -\dfrac{D^\beta}{RT}\varphi c^\beta \nabla\mu^\beta, & \beta = +,-, \\
\multicolumn{4}{l}{\textbf{Secondary Equations}} \\
\hline
\varphi &=& 1-(1-\varphi_0)(1-\nabla\cdot\mathbf{u}) & \\
c^{fc} &=& c_0^{fc}\left(1-\dfrac{\nabla\cdot\mathbf{u}}{\varphi_0}\right) & \\
c^\beta &=& -\dfrac{1}{2z^\beta}z^{fc}c^{fc} + & \\
&+& \dfrac{1}{2}\sqrt{(z^{fc}c^{fc})^2 + \dfrac{4c^2}{f^+f^-}\exp\dfrac{\mu^+ - \mu_0^+ + \mu^- - \mu_0^-}{RT}}, & \\
p &=& \mu^l - \mu_0^l + RT\left(\Gamma^+c^+ + \Gamma^-c^-\right), & \\
\xi &=& \dfrac{1}{z^\beta F}\left(\mu^\beta - \mu_0^\beta - RT\ln\dfrac{f^\beta c^\beta}{c}\right), & \beta = +,-, \\
\multicolumn{4}{l}{\textbf{Boundary Conditions}} \\
\hline
\mathbf{u} &=& \mathbf{0} & \text{on } \Gamma_{\mathbf{u}}^D\times(0,T], \\
\mu^l &=& \mu_{in}^l & \text{on } \Gamma_p^D\times(0,T], \\
\mu^+ &=& \mu_{in}^+ & \text{on } \Gamma_p^D\times(0,T], \\
\mu^- &=& \mu_{in}^- & \text{on } \Gamma_p^D\times(0,T], \\
\mathbf{g}_{\mathbf{u}}^N &=& \mathbf{n}\cdot(\boldsymbol{\sigma}(\mathbf{u}) - p) & \text{on } \Gamma_{\mathbf{u}}^N\times(0,T], \\
\mathbf{n}\cdot\mathbf{q}^l &=& 0 & \text{on } \Gamma_p^N\times(0,T], \\
\mathbf{n}\cdot\mathbf{q}^+ &=& 0 & \text{on } \Gamma_p^N\times(0,T], \\
\mathbf{n}\cdot\mathbf{q}^- &=& 0 & \text{on } \Gamma_p^N\times(0,T].
\end{array}
\tag{2.7.7}
$$

2.8 Reduction to two-component model

In this section, we shall specialise the results from the four-component theory to a binary mixture of a solid and a fluid. By neglecting the ion contributions and the influence of all electrically charged particles in the four-component model, the so-

called two-component mixture model, (is also known in literature as the biphasic model) is derived (Biot, 1941) and (Biot, 1972).

Note that in this case the electroneutrality condition (2.2.11) is not used anymore. Furthermore, the ions conservation (2.4.4) and Fick's law in (2.4.10) disappear. Darcy's law in (2.4.10) is simplified by removing the concentration dependent terms. Therefore, we have

Conservation Equations

$$\begin{aligned} \mathbf{0} &= \nabla \cdot \boldsymbol{\sigma} - \nabla p, \\ 0 &= \frac{\partial \nabla \cdot \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{q}^l, \end{aligned}$$

Constitutive Equations

$$\begin{aligned} \boldsymbol{\sigma} &= 2\mu_s \boldsymbol{\mathcal{E}} + \lambda_s \mathrm{tr}\boldsymbol{\mathcal{E}}, \quad \boldsymbol{\mathcal{E}} = \frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u}^T)), \\ \mathbf{q}^l &= -K \nabla p, \end{aligned}$$

Secondary Equation

$$\varphi = 1 - (1 - \varphi_0)(1 - \nabla \cdot \mathbf{u})$$

Boundary Conditions

$$\begin{aligned} \mathbf{u} &= \mathbf{0} && \text{on } \Gamma_{\mathbf{u}}^D \times (0, T], \\ p &= 0 && \text{on } \Gamma_p^D \times (0, T], \\ \mathbf{g}_{\mathbf{u}}^N &= \mathbf{n} \cdot (\boldsymbol{\sigma}(\mathbf{u}) - p) && \text{on } \Gamma_{\mathbf{u}}^N \times (0, T], \\ \mathbf{n} \cdot \mathbf{q}^l &= 0 && \text{on } \Gamma_p^N \times (0, T], \end{aligned}$$

(2.8.1)

2.9 Conclusions

In this chapter the swelling of charged porous media, like hydrated tissues is modelled by means of mixture theory. Considering four components for the mixture, i.e., solid, fluid, cation and anion, we derived a set of balance equations for each component and for the mixture. The Lagrangian form of the second law of thermodynamics completes the set of equations by means of constitutive equations. The equations are rewritten in a Lagrangian description. Such a description is useful in computer-aided solutions. The boundary conditions are given to complete the model. A reduction to infinitesimal deformation simplifies the reduced system and finally we have shown that by neglecting the ions contribution we come up with the well-known Biot system of equations.

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Chapter 3

An analytical solution of incompressible* charged porous media

Cartilaginous tissues are soft hydrated tissues with strong swelling and shrinking properties. This swelling and shrinkage behaviour of cartilaginous tissues is caused by the flow of water that is bound to the charged solid skeleton of porous tissue. The driving mechanism is an interplay of mechanical, chemical and electrical forces. Swelling and shrinkage can be modelled by a four-component mixture theory described in the previous chapter in which the deformable and charged porous medium is saturated with a fluid with dissolved cations and anions.

The solid skeleton and fluid are assumed to be intrinsically incompressible and therefore a non-zero fluid flux divergence gives rise to swelling or shrinkage of the porous medium. Alternatively, a gradient in the fluid pressure, ion concentrations or voltage results in flow of the fluid and ions. To verify the numerical solutions for this model we need to derive a set of analytical solutions for the reduced system of equations.

In earlier work (Meerveld et al., 2003), a set of analytical solutions has been derived to verify the finite element solution of model. However, in mass balances (Meerveld et al., 2003, equation 2), the time derivatives of volume fractions are considered instead of their material time derivatives. This can only be done if the Lagrangian coordinate is considered (cf. 2.4). Also the diagonalisation (Meerveld et al., 2003, equation 36) produces complex eigenvalues, therefore the obtained solution series are no longer valid. In fact, the equations in this case are of hyperbolic type.

In this chapter, we set ourselves the task of resolving this problem and deriving a set of analytical solutions for the one-dimensional four-component model. We follow (Terzaghi, 1923) and (Biot, 1956) to derive a coupled system of diffusion equations. This leads to the analytical solutions for the two-component mixture model and then generates the solution for the four-component model.

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3.1 Analytical solution for the one-dimensional two-component model

In this section we consider the two-component model of solid and fluid (2.8.1). This model has been widely studied for the consolidation problem (Terzaghi, 1923) and (Biot, 1956). A one-dimensional version of this model reads

Conservation Equations

$$
\begin{aligned}
0 &= (2\mu_s + \lambda_s)\frac{\partial^2 u}{\partial y^2} - \frac{\partial p}{\partial y}, \\
0 &= \frac{\partial^2 u}{\partial t \partial y} - K\frac{\partial^2 p}{\partial y^2},
\end{aligned}
$$

Secondary Equation

$$
\varphi = 1 - (1-\varphi_0)(1 - \frac{\partial u}{\partial y}) \tag{3.1.1}
$$

Boundary Conditions

$$
\begin{aligned}
u &= 0 && \text{on } \Gamma_{\mathbf{u}}^D \times (0,T], \\
p &= 0 && \text{on } \Gamma_p^D \times (0,T], \\
\frac{\partial u}{\partial y} - p &= g_u^N && \text{on } \Gamma_{\mathbf{u}}^N \times (0,T], \\
\frac{\partial p}{\partial y} &= 0 && \text{on } \Gamma_p^N \times (0,T].
\end{aligned}
$$

The momentum balance is integrated in the y-coordinate and is equal to

$$
(2\mu_s + \lambda_s)\frac{\partial u}{\partial y} - p = g_u^N. \tag{3.1.2}
$$

In an experiment setup, for consolidation an instantaneous load at $t = t_0$ is considered (Figure 3.1). Therefore

$$
g_u^N(t) = -f_0 \mathcal{H}(t - t_0) \Rightarrow \frac{\partial g_u^N}{\partial t} = -f_0 \delta(t - t_0).
$$

Hence after differentiating (3.1.2) in t we have,

$$
(2\mu_s + \lambda_s)\frac{\partial^2 u}{\partial t \partial y} - \frac{\partial p}{\partial t} = -f_0 \delta(t - t_0). \tag{3.1.3}
$$

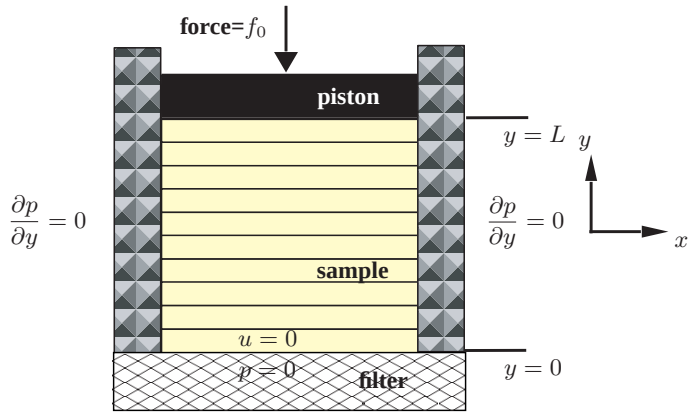

Figure 3.1. Schematic representation of the confined compression experiment.

Substituting this in the mass balance gives

$$\frac{\partial p}{\partial t} = (2\mu_s + \lambda_s)K\frac{\partial^2 p}{\partial y^2} + f_0\delta(t - t_0). \tag{3.1.4}$$

Using separation of variables, the solution of (3.1.4) is given by

$$p(y,t) = \frac{4}{\pi}\sum_{n=0}^{\infty}\frac{1}{2n+1}\sin\left(\frac{2n+1}{2}\frac{\pi}{L}y\right)\exp\left(-\left(\frac{2n+1}{2}\pi\right)^2\frac{(t-t_0)}{C}\right)f_0, \tag{3.1.5}$$

where

$$C = \frac{L^2}{K(2\mu_s + \lambda_s)}.$$

The equations (3.1.2) and (3.1.5) in corporation with the boundary conditions give:

$$u(y,t) = \frac{8L}{(2\mu_s+\lambda_s)\pi^2}\sum_{n=0}^{\infty}\frac{1}{(2n+1)^2}\left(1-\cos\left(\frac{2n+1}{2}\frac{\pi}{L}y\right)\right)\times \left(\exp\left(-\left(\frac{2n+1}{2}\pi\right)^2\frac{(t-t_0)}{C}\right)-1\right)f_0. \tag{3.1.6}$$

Finally the liquid flow q^l is

$$q^l(y,t) = \frac{2K}{L}\sum_{n=0}^{\infty}\cos\left(\frac{2n+1}{2}\frac{\pi}{L}y\right)\exp\left(-\left(\frac{2n+1}{2}\pi\right)^2\frac{(t-t_0)}{C}\right)f_0.$$

A two-dimensional version of the plane stress experiment is considered in detail in (Kaasschieter and Frijns, 2003).

3.2 Analytical solution for the one-dimensional four-component model

Within the concept of mixture theory, we consider a porous solid skeleton and an immiscible pore-fluid. As mentioned in the previous chapter, the solid skeleton and fluid are assumed to be intrinsically incompressible. Assuming infinitesimal deformation for the solid phase, a four-component mixture theory in a Lagrangian description is given in which a charged porous media is saturated with a fluid with dissolved cations and anions (2.7.7).

Following the notations in table 2.1, conservation equations for each constituent implies

$$\boxed{\frac{\partial \Phi^\alpha}{\partial t} + \nabla \cdot (\varphi^\alpha \acute{\mathbf{x}}^{\alpha s}) = 0,\ \alpha = s, l, +, -,} \tag{3.2.1}$$

where $\acute{\mathbf{x}}^{\alpha s} = J\boldsymbol{\mathcal{F}}^{-1}(\mathbf{v}^\alpha - \mathbf{v}^s)$ and $\Phi^\alpha = J\varphi^\alpha$.

The mass flux is measured per unit of area of the reference configuration for the solid phase. Equation (3.2.1) for $\alpha = s$ gives

$$J\varphi^s = \varphi_0^s, \tag{3.2.2}$$

where φ_0^s is the initial volume fraction of solid phase. Equation (3.2.2) together with the saturation assumption implies

$$\varphi^f = 1 - \varphi^s = 1 - \frac{1 - \varphi_0^f}{J}. \tag{3.2.3}$$

Since the solid phase is assumed to have infinitesimal deformation, the Taylor linearisation for J^{-1} at $\boldsymbol{\mathcal{F}} = \mathbf{I}$ implies

$$J^{-1} \approx 1 - \left(\frac{1}{J^2}\frac{\partial J}{\partial \boldsymbol{\mathcal{F}}}\right)\Big|_{F=\mathbf{I}} : (\boldsymbol{\mathcal{F}} - \mathbf{I}) = 1 - \nabla \cdot \mathbf{u},$$

In the above relation, we use $\boldsymbol{\mathcal{F}} = \mathbf{I} + \nabla \mathbf{u}$ and

$$\frac{\partial J}{\partial \boldsymbol{\mathcal{F}}} = J\boldsymbol{\mathcal{F}}^{-T}. \tag{3.2.4}$$

After inserting the linearised form of J^{-1} into (3.2.3) we have

$$\varphi^f = 1 - (1 - \varphi_0^f)(1 - \nabla \cdot \mathbf{u}). \tag{3.2.5}$$

As a consequence of this formula, we have

$$\boxed{\Phi^f = \varphi_0^f + \operatorname{tr} \boldsymbol{\mathcal{E}}(\mathbf{u}).} \tag{3.2.6}$$

Electroneutrality requires

$$z^+ c^+ + z^- c^- + z^{fc} c^{fc} = 0, \tag{3.2.7}$$

where z^β, $\beta = +, -$, is the valence of the dissolved ion β. The superscript 'fc' stands for fixed charge, i.e., the attached ionic group, thus c^{fc} denotes the molar concentration of the attached ions per unit fluid volume.

The conservation of fixed charge in the Lagrangian form reads

$$\varphi^f c^{fc} = \varphi_0^f c_0^{fc} J^{-1}, \tag{3.2.8}$$

where c_0^{fc} is the initial fixed charge concentration. Hence the electroneutrality condition in the initial state takes the following form

$$\frac{z^+\Phi^+}{\overline{V}^+} + \frac{z^-\Phi^-}{\overline{V}^-} + z^{fc}\varphi_0^f c_0^{fc} = 0. \tag{3.2.9}$$

Note that

$$\overline{V}^\beta c^\beta = \frac{\varphi^\beta}{\varphi^f}, \tag{3.2.10}$$

therefore after differentiating in time the electroneutrality condition (3.2.9) can be written as:

$$\boxed{\sum_{\beta=+,-} F\frac{z^\beta}{\overline{V}^\beta}\frac{\partial \Phi^\beta}{\partial t} = \epsilon\frac{\partial \xi}{\partial t},} \tag{3.2.11}$$

where $\epsilon > 0$ is a small departure from electroneutrality. In fact, this assumption is needed for a mathematical reason.

Based on (2.3.32), the constitutive equation to comply the second law of thermodynamics is given by

$$\boxed{-\varphi^\beta \nabla\tilde{\mu}^\beta = \sum_{\gamma=l,+,-} B^{\beta\gamma}\boldsymbol{\mathcal{F}}^T(\mathbf{v}^\gamma - \mathbf{v}^s), \quad \beta = l, +, -,} \tag{3.2.12}$$

where $\tilde{\mu}^l = \mu^l$, $\tilde{\mu}^\beta = \mu^\beta/\overline{V}^\beta$, $\mathbf{B} = (B^{\beta\gamma})_{\beta,\gamma=l,+,-}$, is the friction matrix. Based on (Molenaar et al., 1999), $\mathbf{B}$ is defined as

$$\mathbf{B} = \begin{pmatrix} \dfrac{\varphi^2}{K} + (1-r)^2B^{++} + (1-r)^2B^{--} & -(1-r)B^{++} & -(1-r)B^{--} \\ -(1-r)B^{++} & B^{++} & 0 \\ -(1-r)B^{--} & 0 & B^{--} \end{pmatrix}, \tag{3.2.13}$$

and

$$\tilde{\mu}^l = p + \frac{\partial W}{\partial \Phi}, \tag{3.2.14}$$

$$\tilde{\mu}^\beta = \frac{z^\beta F\xi}{\overline{V}^\beta} + \frac{\partial W}{\partial \Phi^\beta}, \quad \beta = +, -. \tag{3.2.15}$$

In the above relation,

$$B^{\beta\beta} = \varphi^{\beta} RT(\overline{V}^{\beta} D^{\beta})^{-1}, \quad \beta = +, -, \tag{3.2.16}$$

where $D^{\beta} > 0$ is the ion diffusion in free water. $0 \leq r \leq 1$ is the hindrance factor and it is assumed to contain all physical phenomena reducing ionic diffusion rate and identical for cation and anion diffusion. W is the Helmholtz free energy of the porous medium. For such a mixture that consists of four-component, the Helmholtz energy W is expressed as a sum of elastic energy and a mixing energy for β-th constituent, $\beta = l, +, -$, (2.3.30).

$$\begin{aligned} W(\boldsymbol{\mathcal{E}}, \Phi, \Phi^{+}, \Phi^{-}) &= (\mu_0^l + RTc)\Phi + \mu_0^{+}\frac{\Phi^{+}}{\overline{V}^{+}} + \mu_0^{-}\frac{\Phi^{-}}{\overline{V}^{-}} \\ &+ RT(\Phi c - \frac{\Phi^{+}}{\overline{V}^{+}} - \frac{\Phi^{-}}{\overline{V}^{-}}) \left(\ln \frac{\Phi c - \dfrac{\Phi^{+}}{\overline{V}^{+}} - \dfrac{\Phi^{-}}{\overline{V}^{-}}}{\Phi c} - 1 \right) \\ &+ RT\Gamma^{+}\frac{\Phi^{+}}{\overline{V}^{+}} \left(\ln \frac{\Phi^{+}}{\Phi c \overline{V}^{+}} - 1 \right) \\ &+ RT\Gamma^{-}\frac{\Phi^{-}}{\overline{V}^{-}} \left(\ln \frac{\Phi^{-}}{\Phi c \overline{V}^{-}} - 1 \right) + W_E(\boldsymbol{\mathcal{E}}). \end{aligned} \tag{3.2.17}$$

In this relation:

- μ_0^l is the initial electro-chemical potential of the fluid phase,
- μ_0^{β} is the initial electro-chemical potential of ion β,
- $\Gamma^{\beta} \in (0, 1]$ is the osmotic coefficient of cation and anion for $\beta = +, -$, respectively which is uniform and constant. Here we assume $\Gamma^{+} = \Gamma^{-}$ and we denote it by Γ.
- c is the molar concentration of the fluid phase. Since ion concentrations are small, c is assumed to be uniform and constant,
- λ_s and μ_s are the Lamé stress constants,
- R is the universal gas constant,
- T is the absolute temperature, which is uniform and constant, since the state is assumed to be isothermal,
- W_E is the elastic energy and is defined by

$$W_E(\boldsymbol{\mathcal{E}}) = \frac{\lambda_s}{2}(\text{tr}\, \boldsymbol{\mathcal{E}}(\mathbf{u}))^2 + \mu_s \boldsymbol{\mathcal{E}}(\mathbf{u}) : \boldsymbol{\mathcal{E}}(\mathbf{u}). \tag{3.2.18}$$

With the prescribed energy W, the relations (3.2.14) and (3.2.15) are postulated as

$$\tilde{\mu}^l = \tilde{\mu}_0^l + p - RT\Gamma(c^+ + c^-), \tag{3.2.19}$$

$$\tilde{\mu}^\beta = \tilde{\mu}_0^\beta + \frac{z^\beta F\xi}{\overline{V}^\beta} + \frac{RT\Gamma}{\overline{V}^\beta}\ln\frac{c^\beta}{c}, \quad \beta = +,-. \tag{3.2.20}$$

Remark 3.1. *It is easy to see that from* (3.2.7), (3.2.19) *and* (3.2.20) *we have*

$$c^\beta = -\frac{1}{2z^\beta}z^{fc}c^{fc} + \frac{1}{2}\sqrt{(z^{fc}c^{fc})^2 + 4c^2\exp\frac{\overline{V}^+(\tilde{\mu}^+ - \tilde{\mu}_0^+) + \overline{V}^-(\tilde{\mu}^- - \tilde{\mu}_0^-)}{RT\Gamma}}, \tag{3.2.21}$$

for $\beta = +,-$, *and*

$$p = \tilde{\mu}^l - \tilde{\mu}_0^l + RT\Gamma(c^+ + c^-), \tag{3.2.22}$$

$$\xi = \frac{\overline{V}^\beta}{z^\beta F}\left(\tilde{\mu}^\beta - \tilde{\mu}_0^\beta - p - \frac{RT\Gamma}{\overline{V}^\beta}\ln\frac{c^\beta}{c}\right), \quad \beta = +,-. \tag{3.2.23}$$

The above formulas will be needed to derive initial and boundary values for c^β, p *and* ξ.

In the following lemma, we will show that the matrix $\mathbf{B}$ is symmetric positive definite.

Lemma 3.2. $\mathbf{B}$ *is a symmetric positive definite matrix.*

Proof. The symmetry property is trivial. Define the diagonal matrix

$$\mathbf{D} = \text{diag}(1-r, 1, 1),$$

then

$$\mathbf{D}^{-1}\mathbf{B}\mathbf{D}^{-1} = \begin{pmatrix} \dfrac{(\varphi^l)^2}{(1-r)^2K} + B^{++} + B^{--} & -B^{++} & -B^{--} \\ -B^{++} & B^{++} & 0 \\ -B^{--} & 0 & B^{--} \end{pmatrix}. \tag{3.2.24}$$

The diagonal elements of $\mathbf{D}^{-1}\mathbf{B}\mathbf{D}^{-1}$ are all positive and the absolute value of each diagonal element is greater than or equal to the sum of absolute values of the non-diagonal elements in its row (greater in the first row), therefore $\mathbf{D}^{-1}\mathbf{B}\mathbf{D}^{-1}$ is an irreducible diagonally dominant matrix, hence $\mathbf{D}^{-1}\mathbf{B}\mathbf{D}^{-1}$ is positive definite. This is enough to prove the positive definiteness of the matrix $\mathbf{B}$. ■

Note that from equation (3.2.12), we can obtain a relation for the fluxes as:

$$\boxed{\varphi^\beta \acute{\mathbf{x}}^{\beta s} = -\sum_{\gamma=l,+,-}\mathbf{P}^{\beta\gamma}\nabla\tilde{\mu}^\gamma, \quad \beta = l,+,-,} \tag{3.2.25}$$

where $\mathbf{P} = J\mathbf{N}(\boldsymbol{\mathcal{F}}^T\mathbf{B}\boldsymbol{\mathcal{F}})^{-1}\mathbf{N}$ and $\mathbf{N} = \text{diag}(\varphi^l, \varphi^+, \varphi^-)$.

Remark 3.3. *Since the determinant of the deformation gradient $\boldsymbol{\mathcal{F}}$ is positive, based on Lemma 3.2,* $\mathbf{B}$ *is a symmetric positive definite matrix. Therefore* $\mathbf{P}$ *is a symmetric positive definite matrix too.*

Differentiating the equations (3.2.14) and (3.2.15) in time and using the fact that the energy function $W = W(\boldsymbol{\mathcal{E}}, \Phi, \Phi^+, \Phi^-)$ gives:

$$\frac{\partial}{\partial t}(\tilde{\mu}^l - p) = \frac{\partial}{\partial \Phi}\left[\frac{\partial W}{\partial \boldsymbol{\mathcal{E}}} : \frac{\partial \boldsymbol{\mathcal{E}}}{\partial t} + \sum_{\gamma=l,+,-} \frac{\partial W}{\partial \Phi^\gamma}\frac{\partial \Phi^\gamma}{\partial t}\right], \tag{3.2.26}$$

$$\frac{\partial}{\partial t}\left(\tilde{\mu}^\beta - \frac{z^\beta F \xi}{\overline{V}^\beta}\right) = \frac{\partial}{\partial \Phi^\beta}\left[\frac{\partial W}{\partial \boldsymbol{\mathcal{E}}} : \frac{\partial \boldsymbol{\mathcal{E}}}{\partial t} + \sum_{\gamma=l,+,-} \frac{\partial W}{\partial \Phi^\gamma}\frac{\partial \Phi^\gamma}{\partial t}\right],\ \beta = +,-. \tag{3.2.27}$$

Observation of (3.2.17) reveals that the first terms on the right-hand sides of the preceding two equations vanishes. This results into

$$\frac{\partial}{\partial t}(\tilde{\mu}^l - p) = \sum_{\gamma=l,+,-} W^{l\gamma}\frac{\partial \Phi^\gamma}{\partial t}, \tag{3.2.28}$$

$$\frac{\partial}{\partial t}\left(\tilde{\mu}^\beta - \frac{z^\beta F \xi}{\overline{V}^\beta}\right) = \sum_{\gamma=l,+,-} W^{\beta\gamma}\frac{\partial \Phi^\gamma}{\partial t},\ \beta = +,-, \tag{3.2.29}$$

where $W^{\beta\gamma} = \dfrac{\partial^2 W}{\partial \Phi^\beta \partial \Phi^\gamma}$ and $\mathbf{W} = (W^{\beta\gamma})_{\beta,\gamma=l,+,-}$.

Note that $\mathbf{W}$ is a symmetric positive semi-definite matrix, indeed, from (3.2.19) and (3.2.20), the matrix $\mathbf{W}$ is of the form

$$\mathbf{W} = RT\Gamma \begin{pmatrix} \dfrac{1}{\Phi^2}\left(\dfrac{\Phi^+}{\overline{V}^+} + \dfrac{\Phi^-}{\overline{V}^-}\right) & -\dfrac{1}{\Phi\overline{V}^+} & -\dfrac{1}{\Phi\overline{V}^-} \\ -\dfrac{1}{\Phi\overline{V}^+} & \dfrac{1}{\Phi^+\overline{V}^+} & 0 \\ -\dfrac{1}{\Phi\overline{V}^-} & 0 & \dfrac{1}{\Phi^-\overline{V}^-} \end{pmatrix}. \tag{3.2.30}$$

Define the diagonal matrix $\tilde{\mathbf{N}} = \text{diag}\,(\Phi, \Phi^+, \Phi^-)$, then

$$\tilde{\mathbf{N}}\mathbf{W}\tilde{\mathbf{N}} = RT\Gamma \begin{pmatrix} \dfrac{\Phi^+}{\overline{V}^+} + \dfrac{\Phi^-}{\overline{V}^-} & -\dfrac{\Phi^+}{\overline{V}^+} & -\dfrac{\Phi^-}{\overline{V}^-} \\ -\dfrac{\Phi^+}{\overline{V}^+} & \dfrac{\Phi^+}{\overline{V}^+} & 0 \\ -\dfrac{\Phi^-}{\overline{V}^-} & 0 & \dfrac{\Phi^-}{-\overline{V}^-} \end{pmatrix}. \tag{3.2.31}$$

It is easy to see that $\tilde{\mathbf{N}}\mathbf{W}\tilde{\mathbf{N}}$ is symmetric positive semi-definite of rank two with zero eigenvectors $(1,1,1)^T$. Thus, $\mathbf{W}$ is symmetric positive semi-definite of rank two.

The preceding relations can be written as:

$$\mathbf{W}\frac{\partial}{\partial t}\begin{pmatrix}\Phi\\ \Phi^+\\ \Phi^-\end{pmatrix} = \frac{\partial}{\partial t}\begin{pmatrix}\tilde{\mu}^l\\ \tilde{\mu}^+\\ \tilde{\mu}^-\end{pmatrix} - \mathbf{F}\frac{\partial}{\partial t}\begin{pmatrix}p\\ \xi\end{pmatrix}, \tag{3.2.32}$$

where

$$\mathbf{F} = \begin{pmatrix}1 & 0\\ 0 & \frac{Fz^+}{\overline{V}^+}\\ 0 & \frac{Fz^-}{\overline{V}^-}\end{pmatrix}. \tag{3.2.33}$$

In order to solve the above system of equations, we need to pose boundary conditions. This can be achieved by suitably combining the essential conditions for $\tilde{\mu}^l$, $\tilde{\mu}^+$, $\tilde{\mu}^-$ and $\mathbf{u}$ and the natural conditions for the normal components of $\dot{\mathbf{x}}^{\beta s}$, $(\beta = l,+,-)$ and $\boldsymbol{\sigma}$.

Consider the case that the porous medium is in contact with an electro-neutral bathing solution, given that the pressure p_{out}, the voltage ξ_{out} and the ion concentrations c_{out} are known. The bathing solution contains no fixed charges, thus $c^+_{out} = c^-_{out} = c_{out}$. Since the electro-chemical potentials are continuous at the boundary (Huyghe and Janssen, 1997),

$$\tilde{\mu}^l_{in} = \tilde{\mu}^l_{out}, \tag{3.2.34}$$
$$\tilde{\mu}^+_{in} = \tilde{\mu}^+_{out}, \tag{3.2.35}$$
$$\tilde{\mu}^-_{in} = \tilde{\mu}^-_{out}, \tag{3.2.36}$$

where $\tilde{\mu}^l_{out}$ and $\tilde{\mu}^\beta_{out}$ are the electro-chemical potentials in the outer solution. Assume $\Gamma^+_{in} = \Gamma^-_{in} = \Gamma$ and $\Gamma^+_{out} = \Gamma^-_{out} = 1$, then the combination of the above relations and the relations expressed in (3.2.19) and (3.2.20) provides

$$\pi = p_{in} - p_{out} = RT\Gamma(c^+_{in} + c^-_{in}) - 2RTc_{out}, \tag{3.2.37}$$

and

$$\frac{c^2_{out}}{c^2} = \left(\frac{c^+_{in}c^-_{in}}{c^2}\right)^\Gamma, \tag{3.2.38}$$
$$\xi_{in} - \xi_{out} = \frac{RT}{Fz^\beta}\ln\frac{c_{out}c^{\Gamma-1}}{(c^\beta_{in})^\Gamma}, \quad \beta = +,-, \tag{3.2.39}$$

In (3.2.37), π is the osmotic pressure (Richards, 1980). In (3.2.39), $\xi_{in} - \xi_{out}$ describes the jump on the electrical potential. It is called the Nernst potential, e.g. (Gu et .al, 1999) and (Helfferich, 1962). By using the electroneutrality condition (3.2.7), we derive the Donnan equilibrium concentration of ions as

$$c^\beta_{in} = -\frac{1}{2z^\beta}z^{fc}c^{fc} + \frac{1}{2}\sqrt{\left(z^{fc}c^{fc}\right)^2 + 4f^+f^-c^2_{out}}, \quad \beta = +,-, \tag{3.2.40}$$

where

$$f^{\beta} = \left(\frac{c^{\beta}}{c}\right)^{\Gamma-1}, \quad \beta = +, -.$$

Using (3.2.18)-(3.2.19) we can derive the boundary values for the electro-chemical potentials $\tilde{\mu}^{l}_{in}$ and $\tilde{\mu}^{\beta}_{in}$ as

$$\tilde{\mu}^{l}_{in} = \tilde{\mu}^{l}_{0} + p_{out} - 2RTc_{out}, \tag{3.2.41}$$

$$\tilde{\mu}^{\beta}_{in} = \tilde{\mu}^{\beta}_{0} + p_{out} + \frac{Fz^{\beta}}{\overline{V}^{\beta}}\xi_{out} + \frac{RT}{\overline{V}^{\beta}}\ln\frac{c_{out}}{c}, \quad \beta = +, -. \tag{3.2.42}$$

We can summarize all the above statements to the following boundary conditions:

$$\begin{aligned}
\mathbf{u} &= \mathbf{0} && \text{on } (\partial\Omega_{t_0})^{D}_{\mathbf{u}} \times (0,T], && \text{(3.2.43a)}\\
\tilde{\mu}^{l} &= \tilde{\mu}^{l}_{in} && \text{on } (\partial\Omega_{t_0})^{D}_{p} \times (0,T], && \text{(3.2.43b)}\\
\tilde{\mu}^{+} &= \tilde{\mu}^{+}_{in} && \text{on } (\partial\Omega_{t_0})^{D}_{p} \times (0,T], && \text{(3.2.43c)}\\
\tilde{\mu}^{-} &= \tilde{\mu}^{-}_{in} && \text{on } (\partial\Omega_{t_0})^{D}_{p} \times (0,T], && \text{(3.2.43d)}\\
\mathbf{n}\cdot(\boldsymbol{\sigma}(\mathbf{u}) - p) &= \mathbf{g}^{N}_{\mathbf{u}} && \text{on } (\partial\Omega_{t_0})^{N}_{\mathbf{u}} \times (0,T], && \text{(3.2.43e)}\\
\mathbf{n}\cdot\mathbf{q} &= 0 && \text{on } (\partial\Omega_{t_0})^{N}_{p} \times (0,T], && \text{(3.2.43f)}\\
\mathbf{n}\cdot\mathbf{q}^{+} &= 0 && \text{on } (\partial\Omega_{t_0})^{N}_{p} \times (0,T], && \text{(3.2.43g)}\\
\mathbf{n}\cdot\mathbf{q}^{-} &= 0 && \text{on } (\partial\Omega_{t_0})^{N}_{p} \times (0,T], && \text{(3.2.43h)}
\end{aligned}$$

where the sets $(\partial\Omega_{t_0})^{D}_{\mathbf{u}}$ and $(\partial\Omega_{t_0})^{N}_{\mathbf{u}}$ (and similarly $(\partial\Omega_{t_0})^{D}_{p}$ and $(\partial\Omega_{t_0})^{N}_{p}$) to be two disjoint open subsets of the total boundary $\partial\Omega_{t_0}$, such that $(\partial\Omega_{t_0})^{D}_{\alpha} \cap (\partial\Omega_{t_0})^{N}_{\alpha} = \emptyset$ and $(\partial\Omega_{t_0})^{D}_{\alpha} \cup (\partial\Omega_{t_0})^{N}_{\alpha} = \partial\Omega_{t_0}$ for $\alpha = \mathbf{u}$ and p.

3.2.1 One-dimensional configuration

In this section, we reduce the total set of equation to a one dimensional configuration. The momentum balance in (2.8.1):

$$(2\mu_s + \lambda_s)\frac{\partial^2 u}{\partial x^2} - \frac{\partial p}{\partial x} = 0. \tag{3.2.44}$$

Following Terzaghi (Terzaghi, 1923), the momentum balance equation is integrated in the x-coordinate into

$$\boxed{(2\mu_s + \lambda_s)\frac{\partial u}{\partial x} - (p - p_{in}) = g^{N}_{u},} \tag{3.2.45}$$

where g_u^N from (3.2.43e) is the external load on the sample. In the experimental setup, for consolidation an instantaneous mechanical loading at $t = t_0$ is considered and the external mechanical loading remains unaltered for free swelling. Therefore,

$$g_u^N(t) = -f_0\mathcal{H}(t-t_0) \Rightarrow \frac{\partial g_u^N(t)}{\partial t} = -f_0\delta(t-t_0).$$

After differentiating (3.2.45) in t, we have

$$(2\mu_s + \lambda_s)\frac{\partial}{\partial t}\frac{\partial u}{\partial x} - \frac{\partial p}{\partial t} = -f_0\delta(t-t_0). \tag{3.2.46}$$

The one-dimensional form of equation (3.2.6) gives $\Phi = \varphi_0^f + \dfrac{\partial u}{\partial x}$. Differentiating with respect to time gives

$$\frac{\partial \Phi}{\partial t} = \frac{\partial}{\partial t}\frac{\partial u}{\partial x}. \tag{3.2.47}$$

Then (3.2.46) converts to

$$\frac{1}{2\mu_s + \lambda_s}\frac{\partial p}{\partial t} - \frac{\partial \Phi}{\partial t} = \frac{f_0}{2\mu_s + \lambda_s}\delta(t-t_0). \tag{3.2.48}$$

Combining this equation and the electroneutrality equation (3.2.11) results into:

$$\mathbf{H}_\epsilon \frac{\partial}{\partial t}\begin{pmatrix} p \\ \xi \end{pmatrix} = \mathbf{F}^T \frac{\partial}{\partial t}\begin{pmatrix} \Phi \\ \Phi^+ \\ \Phi^- \end{pmatrix} + \frac{f_0\delta(t-t_0)}{2\mu_s + \lambda_s}\begin{pmatrix} 1 \\ 0 \end{pmatrix}, \tag{3.2.49}$$

where

$$\mathbf{H}_\epsilon = \begin{pmatrix} 1/(2\mu_s + \lambda_s) & 0 \\ 0 & \epsilon \end{pmatrix}. \tag{3.2.50}$$

In this part, we assume that the matrix $\mathbf{P}$ is constant. In fact, this assumption is made to linearise the problem. After substituting the constitutive equation (3.2.25) in the balance equation (3.2.1), we derive the following relation between Φ^β and $\tilde{\mu}^\beta$

$$\frac{\partial}{\partial t}\begin{pmatrix} \Phi \\ \Phi^+ \\ \Phi^- \end{pmatrix} = \mathbf{P}\frac{\partial^2}{\partial x^2}\begin{pmatrix} \tilde{\mu}^l \\ \tilde{\mu}^+ \\ \tilde{\mu}^- \end{pmatrix}. \tag{3.2.51}$$

Now (3.2.32), (3.2.49) and (3.2.51) imply that

$$\frac{\partial}{\partial t}\begin{pmatrix} \tilde{\mu}^l \\ \tilde{\mu}^+ \\ \tilde{\mu}^- \end{pmatrix} = \left(\mathbf{W} + \mathbf{F}\mathbf{H}_\epsilon^{-1}\mathbf{F}^T\right)\mathbf{P}\frac{\partial^2}{\partial x^2}\begin{pmatrix} \tilde{\mu}^l \\ \tilde{\mu}^+ \\ \tilde{\mu}^- \end{pmatrix} + f_0\delta(t-t_0)\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}. \tag{3.2.52}$$

If we define

$$\mathbf{E} = \mathbf{W} + \mathbf{F}\mathbf{H}_\epsilon^{-1}\mathbf{F}^T, \tag{3.2.53}$$

the previous equation can be written as:

$$\boxed{\frac{\partial}{\partial t}\begin{pmatrix}\tilde{\mu}^l\\ \tilde{\mu}^+\\ \tilde{\mu}^-\end{pmatrix} = \mathbf{EP}\frac{\partial^2}{\partial x^2}\begin{pmatrix}\tilde{\mu}^l\\ \tilde{\mu}^+\\ \tilde{\mu}^-\end{pmatrix} + f_0\delta(t-t_0)\begin{pmatrix}1\\ 0\\ 0\end{pmatrix}.} \tag{3.2.54}$$

Lemma 3.4. $\mathbf{E}$ *is a symmetric positive definite matrix.*

Proof. It has been shown that $\mathbf{W}$ is symmetric positive semi-definite of rank two with zero eigenvector $(\Phi, \Phi^+, \Phi^-)^T$. On the other hand, matrix $\mathbf{F}\mathbf{H}_\epsilon^{-1}\mathbf{F}^T$ with zero eigenvector $\left(0, \frac{Fz^-}{\overline{V}^-}, -\frac{Fz^+}{\overline{V}^+}\right)^T$ is symmetric positive semi-definite of rank two. Therefore $\mathbf{E}$ is symmetric positive definite. ■

In the next step, we modify the coupled system (3.2.54) by using the above lemma. Since $\mathbf{E}^{-1}$ is a symmetric positive definite matrix, it can be decomposed into $\mathbf{E}^{-1} = \mathbf{G}^T\mathbf{G}$, where $\mathbf{G}$ is a non-singular matrix. The matrix $\mathbf{A} = \mathbf{G}^{-T}\mathbf{P}\mathbf{G}^{-1}$ is symmetric positive definite, thus it decomposes as $\mathbf{A} = \mathbf{M}\mathbf{\Lambda}\mathbf{M}^{-1}$ where $\mathbf{M}$ is a non-singular matrix corresponding to the eigenvectors of $\mathbf{A}$, and $\mathbf{\Lambda}$ a diagonal matrix corresponding to the eigenvalues of $\mathbf{A}$. Define $\mathbf{M}_1 = \mathbf{G}^{-1}\mathbf{M}$ and

$$\begin{pmatrix}\eta^l\\ \eta^+\\ \eta^-\end{pmatrix} = \mathbf{M}_1^{-1}\begin{pmatrix}\tilde{\mu}^l\\ \tilde{\mu}^+\\ \tilde{\mu}^-\end{pmatrix}, \tag{3.2.55}$$

then the coupled system (3.2.54) can be modified into:

$$\boxed{\frac{\partial \eta^\beta}{\partial t} = \lambda^\beta \frac{\partial^2 \eta^\beta}{\partial x^2} + g(t), \quad \beta = l, +, -,} \tag{3.2.56}$$

with

$$g(t) = f_0 \sum_{\gamma=l,+,-} M^{\beta\gamma}\delta(t-t_0), \tag{3.2.57}$$

where $\mathbf{M} = (M^{\beta\gamma})_{\beta,\gamma=l,+,-}$.

3.2.2 Consolidation and free swelling experiments

In this section, the analytical solutions are derived for consolidation, free swelling. We assume constant material parameters and small deformation with respect to an initial steady reference state at $t = t_0$. The homogeneous sample is placed frictionless in a holder. Figure 3.2 illustrates the experimental setup. At the bottom $x = 0$, the sample is in contact with a glass filter saturated by a sodium chloride solution. An impermeable piston is placed on the top of the sample, $x = L$, where an external mechanical load is applied. The sample was made out of a hydrogel. A bathing solution flowed through a porous glass filter at the bottom of the sample.

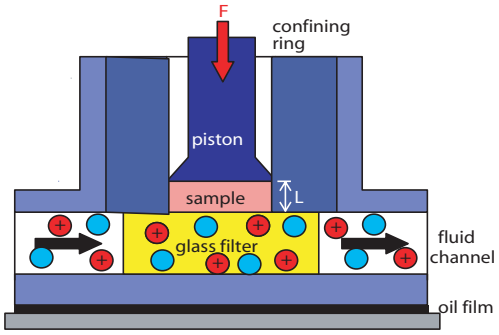

Figure 3.2. Schematic representation of the experimental set-up

Consolidation

In the consolidation experiment, we apply a load on the piston to be equal to $f(t) = -f_0\mathcal{H}(t-t_0)$, with $\mathcal{H}(t-t_0)$ the Heaviside function and $f_0 > 0$. We assume a sufficiently small value for f_0 to ensure that $\mathbf{W}$ and $\mathbf{P}$ are constant in time. For the reference values of electro-chemical potentials we choose

$$\tilde{\mu}_0^l = 2RTc_{out}, \quad \tilde{\mu}_0^\beta = -\frac{RT}{\overline{V}^\beta}\ln\frac{c_{out}}{c}. \tag{3.2.58}$$

Now from (3.2.34)-(3.2.36) and assuming that $p_{out} = 0$ and $\xi_{out} = 0$, we obtain zero values for the inner electro-chemical potentials, i.e., $\tilde{\mu}_{in}^\beta = 0$, $\beta = l, +, -$.
The initial and boundary conditions for the displacement, fluid pressure, electrical potential and electro-chemical potentials with respect to the steady reference state $t = t_0$ are:

$$\begin{aligned}
\left[\begin{array}{ccc}\tilde{\mu}^l & \tilde{\mu}^+ & \tilde{\mu}^-\end{array}\right](0,t) &= \left[\begin{array}{ccc}0 & 0 & 0\end{array}\right],\\
\frac{\partial}{\partial x}\left[\begin{array}{ccc}\tilde{\mu}^l & \tilde{\mu}^+ & \tilde{\mu}^-\end{array}\right](L,t) &= \left[\begin{array}{ccc}0 & 0 & 0\end{array}\right],\\
\left[\begin{array}{ccc}\tilde{\mu}^l & \tilde{\mu}^+ & \tilde{\mu}^-\end{array}\right](x,t_0) &= \left[\begin{array}{ccc}\tilde{\mu}_{t_0}^l & \tilde{\mu}_{t_0}^+ & \tilde{\mu}_{t_0}^-\end{array}\right],\\
\left[\begin{array}{ccc}p & \xi & u\end{array}\right](0,t) &= \left[\begin{array}{ccc}p_{in} & \xi_{in} & 0\end{array}\right],\\
\left[\begin{array}{ccc}p & \xi & u\end{array}\right](x,t_0) &= \left[\begin{array}{ccc}p_{t_0} & \xi_{t_0} & 0\end{array}\right],
\end{aligned}$$

where $\left[\begin{array}{ccc}\tilde{\mu}_{t_0}^l & \tilde{\mu}_{t_0}^+ & \tilde{\mu}_{t_0}^-\end{array}\right] = \left[\begin{array}{ccc}f_0 & 0 & 0\end{array}\right]$.

In fact assuming the above initial condition, we attempt to solve the system (3.2.56) with $g(t) = 0$.

Given $\tilde{\mu}_{in}^\beta$ and $\tilde{\mu}_{t_0}^\beta$, $(\beta = l, +, -)$, the values of $[p_{in}\,\xi_{in}]$ and $[p_{t_0}\,\xi_{t_0}]$ respectively can be calculated by Remark 3.1.

The method of separation of variables is applied to solve (3.2.56) in correspond-

ing with the boundary and initial conditions. The solutions are:

$$\begin{pmatrix} \tilde{\mu}^l(x,t) \\ \tilde{\mu}^+(x,t) \\ \tilde{\mu}^-(x,t) \end{pmatrix} = \frac{4}{\pi}\sum_{n=0}^{\infty}\frac{1}{2n+1}\sin\left(\frac{2n+1}{2}\frac{\pi}{L}x\right)\mathbf{M}_1\mathbf{R}_n\mathbf{M}_1^{-1}\begin{pmatrix} \tilde{\mu}^l_{t_0} \\ \tilde{\mu}^+_{t_0} \\ \tilde{\mu}^-_{t_0} \end{pmatrix}, \tag{3.2.59}$$

in which $\mathbf{R}_n$ is a diagonal matrix with

$$\mathbf{R}_n^{ii} = \exp\left(-\left(\frac{2n+1}{2}\pi\right)^2\frac{\lambda_i(t-t_0)}{L^2}\right), \quad i = l,+,-. \tag{3.2.60}$$

Using relation (3.2.49), (3.2.51) and (3.2.54) and after time integration we have

$$\begin{aligned}\begin{pmatrix} p \\ \xi \end{pmatrix} &= \mathbf{H}_\epsilon^{-1}\mathbf{F}^T\mathbf{E}^{-1}\begin{pmatrix} \tilde{\mu}^l(x,t) \\ \tilde{\mu}^+(x,t) \\ \tilde{\mu}^-(x,t) \end{pmatrix} - \mathbf{H}_\epsilon^{-1}\mathbf{F}^T\mathbf{E}^{-1}f_0\mathcal{H}(t-t_0)\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \\ &+ \mathbf{H}_\epsilon^{-1}f_0\frac{\mathcal{H}(t-t_0)}{2\mu_s+\lambda_s}\begin{pmatrix} 1 \\ 0 \end{pmatrix} + f_1(x).\end{aligned}$$

By using the initial condition for p and ξ at $t = t_0^+$, the function $f_1(x)$ is equal to

$$f_1(x) = \begin{pmatrix} p_{t_0} \\ \xi_{t_0} \end{pmatrix} - \begin{pmatrix} f_0 \\ 0 \end{pmatrix}.$$

Therefore we have

$$\begin{pmatrix} p \\ \xi \end{pmatrix} = \mathbf{H}_\epsilon^{-1}\mathbf{F}^T\mathbf{E}^{-1}\begin{pmatrix} \tilde{\mu}^l(x,t) - \tilde{\mu}^l_{t_0} \\ \tilde{\mu}^+(x,t) - \tilde{\mu}^+_{t_0} \\ \tilde{\mu}^-(x,t) - \tilde{\mu}^-_{t_0} \end{pmatrix} + \begin{pmatrix} p_{t_0} \\ \xi_{t_0} \end{pmatrix}.$$

By plugging equation (3.2.59) into the above identity we obtain

$$\begin{aligned}\begin{pmatrix} p(x,t) \\ \xi(x,t) \end{pmatrix} &= \mathbf{H}_\epsilon^{-1}\mathbf{F}^T\mathbf{E}^{-1}\frac{4}{\pi}\sum_{n=0}^{\infty}\frac{1}{2n+1}\times \\ &\sin\left(\frac{2n+1}{2}\frac{\pi}{L}\mathbf{x}\right)\mathbf{M}_1(\mathbf{R}_n - \mathbf{I})\mathbf{M}_1^{-1}\begin{pmatrix} \tilde{\mu}^l_{t_0} \\ \tilde{\mu}^+_{t_0} \\ \tilde{\mu}^-_{t_0} \end{pmatrix} + \begin{pmatrix} p_{t_0} \\ \xi_{t_0} \end{pmatrix}.\end{aligned} \tag{3.2.61}$$

After integration in space of equations (3.2.45) we have

$$u(x,t) = \frac{1}{2\mu_s+\lambda_s}\int_0^x (p - p_{in})\,dx - f_0\mathcal{H}(t-t_0)x + f_2(t).$$

Assuming $x = 0$ and considering the boundary condition $u(0,t) = 0$, we obtain $f_2(t) = 0$. Let $t = t_0^+$, then we have

$$p_{t_0} = p_{in} - f_0.$$

Using the above fact and plugging (3.2.61) into the relation for u,

$$u(x,t) = \frac{1}{2\mu_s + \lambda_s} \begin{pmatrix} 1 & 0 \end{pmatrix} \mathbf{H}_\epsilon^{-1} \mathbf{F}^T \mathbf{E}^{-1} \frac{8L}{\pi^2} \sum_{n=0}^{\infty} \frac{1}{(2n+1)^2} \times \left(1 - \cos\left(\frac{2n+1}{2}\frac{\pi}{L}x\right)\right) \mathbf{M}_1 (\mathbf{R}_n - \mathbf{I}) \mathbf{M}_1^{-1} \begin{pmatrix} \tilde{\mu}_{t_0}^l \\ \tilde{\mu}_{t_0}^+ \\ \tilde{\mu}_{t_0}^- \end{pmatrix}. \tag{3.2.62}$$

Given equations (3.2.25) and (3.2.59), the fluxes $\Phi^\beta \dot{\mathbf{x}}^{\beta s}$, $\beta = l, +, -$ are equal to

$$\begin{pmatrix} \varphi \dot{x}^{ls}(x,t) \\ \varphi^+ \dot{x}^{+s}(x,t) \\ \varphi^- \dot{x}^{-s}(x,t) \end{pmatrix} = -\frac{2}{L} \sum_{n=0}^{\infty} \cos\left(\frac{2n+1}{2}\frac{\pi}{L}x\right) \mathbf{P}\mathbf{M}_1 \mathbf{R}_n \mathbf{M}_1^{-1} \begin{pmatrix} \tilde{\mu}_{t_0}^l \\ \tilde{\mu}_{t_0}^+ \\ \tilde{\mu}_{t_0}^- \end{pmatrix}. \tag{3.2.63}$$

Free swelling

In the next experiment, we change the concentration of the external salt solution. Considering the reference values for the electro-chemical potentials to be equal to zero, the equations (3.2.41) and (3.2.42) yields the following boundary and initial conditions for the free swelling experiment:

$$\begin{aligned} \begin{bmatrix} \tilde{\mu}^l & \tilde{\mu}^+ & \tilde{\mu}^- \end{bmatrix}(0,t) &= \begin{bmatrix} \tilde{\mu}_{in}^l & \tilde{\mu}_{in}^+ & \tilde{\mu}_{in}^- \end{bmatrix}, \\ \frac{\partial}{\partial x} \begin{bmatrix} \tilde{\mu}^l & \tilde{\mu}^+ & \tilde{\mu}^- \end{bmatrix}(L,t) &= \begin{bmatrix} 0 & 0 & 0 \end{bmatrix}, \\ \begin{bmatrix} \tilde{\mu}^l & \tilde{\mu}^+ & \tilde{\mu}^- \end{bmatrix}(x,t_0) &= \begin{bmatrix} \tilde{\mu}_{t_0}^l & \tilde{\mu}_{t_0}^+ & \tilde{\mu}_{t_0}^- \end{bmatrix}, \\ \begin{bmatrix} p & \xi & u \end{bmatrix}(0,t) &= \begin{bmatrix} p_{in} & \xi_{in} & 0 \end{bmatrix}, \\ \begin{bmatrix} p & \xi & u \end{bmatrix}(x,t_0) &= \begin{bmatrix} p_{t_0} & \xi_{t_0} & 0 \end{bmatrix}, \end{aligned}$$

in which $\tilde{\mu}_{t_0}^\beta = 0$, $\beta = l, +, -$, and

$$\begin{cases} \tilde{\mu}_{in}^l = & -2RT\Delta c_{out}, \\ \tilde{\mu}_{in}^+ = & \dfrac{RT}{\overline{V}^+} \ln \dfrac{c_{out}(t_0^+)}{c_{out}(t_0^-)}, \\ \tilde{\mu}_{in}^- = & \dfrac{RT}{\overline{V}^-} \ln \dfrac{c_{out}(t_0^+)}{c_{out}(t_0^-)}, \end{cases} \tag{3.2.64}$$

Δc_{out} is the change in the external concentration and t_0^+ and t_0^- are the time just after and before t_0 when chemical loading is applied.

Given $\tilde{\mu}^{\beta}_{in}$ and $\tilde{\mu}^{\beta}_{t_0}$, $\beta = l, +, -$, the values of $[p_{in}\ \xi_{in}]$ and $[p_{t_0}\ \xi_{t_0}]$ respectively can be calculated by Remark 3.1.

The change in the external concentration is considered sufficiently small such that firstly, $\mathbf{W}$ and $\mathbf{P}$ are considered to be constant in time and secondly, the change of the electro-chemical potentials of the ions is approximately linear.

We follow the same outline as in the consolidation experiments to derive the solution of the equation (3.2.56) with the above initial and boundary conditions. This gives

$$\begin{pmatrix} \tilde{\mu}^{l}(x,t) \\ \tilde{\mu}^{+}(x,t) \\ \tilde{\mu}^{-}(x,t) \end{pmatrix} = \left[\mathbf{I} - \frac{4}{\pi}\sum_{n=0}^{\infty}\frac{1}{2n+1}\times \right. \\ \left. \sin\left(\frac{2n+1}{2}\frac{\pi}{L}x\right)\mathbf{M}_1\mathbf{R}_n\mathbf{M}_1^{-1}\right]\begin{pmatrix} \tilde{\mu}^{l}_{in} \\ \tilde{\mu}^{+}_{in} \\ \tilde{\mu}^{-}_{in} \end{pmatrix}, \tag{3.2.65}$$

$$\begin{pmatrix} p(x,t) \\ \xi(x,t) \end{pmatrix} = \mathbf{H}_{\epsilon}^{-1}\mathbf{F}^{T}\mathbf{E}^{-1}\frac{4}{\pi}\sum_{n=0}^{\infty}\frac{1}{2n+1}\times \\ \sin\left(\frac{2n+1}{2}\frac{\pi}{L}x\right)\mathbf{M}_1(\mathbf{I}-\mathbf{R}_n)\mathbf{M}_1^{-1}\begin{pmatrix} \tilde{\mu}^{l}_{in} \\ \tilde{\mu}^{+}_{in} \\ \tilde{\mu}^{-}_{in} \end{pmatrix}, \tag{3.2.66}$$

$$u(x,t) = \frac{1}{2\mu_s+\lambda_s}\begin{pmatrix} 1 & 0 \end{pmatrix}\mathbf{H}_{\epsilon}^{-1}\mathbf{F}^{T}\mathbf{E}^{-1}\frac{8L}{\pi^2}\sum_{n=0}^{\infty}\frac{1}{(2n+1)^2}\times \\ \left(1-\cos\left(\frac{2n+1}{2}\frac{\pi}{L}x\right)\right)\mathbf{M}_1(\mathbf{I}-\mathbf{R}_n)\mathbf{M}_1^{-1}\begin{pmatrix} \tilde{\mu}^{l}_{in} \\ \tilde{\mu}^{+}_{in} \\ \tilde{\mu}^{-}_{in} \end{pmatrix}. \tag{3.2.67}$$

Like the consolidation problem, the fluxes $\acute{\mathbf{x}}^{\beta s}$ are derived and are equal to

$$\begin{pmatrix} \varphi\acute{x}^{ls}(x,t) \\ \varphi^{+}\acute{x}^{+s}(x,t) \\ \varphi^{-}\acute{x}^{-s}(x,t) \end{pmatrix} = \frac{2}{L}\sum_{n=0}^{\infty}\cos\left(\frac{2n+1}{2}\frac{\pi}{L}x\right)\mathbf{P}\mathbf{M}_1\mathbf{R}_n\mathbf{M}_1^{-1}\begin{pmatrix} \tilde{\mu}^{l}_{in} \\ \tilde{\mu}^{+}_{in} \\ \tilde{\mu}^{-}_{in} \end{pmatrix}. \tag{3.2.68}$$

3.2.3 Results

In this section, the results for the consolidation and the free swelling are prescribed. As mentioned in the previous section, an uniaxial confined swelling and compression experiment performed on a cylindrical sample of cartilage substitute. This sample, with the diameter of 4 mm and the height of approximately 1 mm 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 of ion concentrations and electro-chemical potentials as well as pressure and voltage.

During the experiment, the mechanical and chemical load were varied. Inspired by them, two numerical simulations are considered.

For both computations, the parameters in table 3.1 are considered:

Parameter	Unit	Value
$2\mu_s + \lambda_s$	MPa	4×10^3
K	$\mathrm{m}^4\ \mathrm{N}^{-1}\ \mathrm{s}^{-1}$	1.0×10^{-18}
c^{fc}	$\mathrm{mol\ m}^{-3}$	-2×10^2
c_{out}	$\mathrm{mol\ m}^{-3}$	1×10^2
φ		0.2
D^+	$\mathrm{m}^2\ \mathrm{s}^{-1}$	13.3×10^{-10}
D^-	$\mathrm{m}^2\ \mathrm{s}^{-1}$	20.3×10^{-10}
R	$\mathrm{J\ mol}^{-1}\ \mathrm{K}^{-1}$	8.3145
T	K	293
F	$\mathrm{C\ mol}^{-1}$	96484.6
Γ		0.9
ϵ	$\mathrm{C}^2\ \mathrm{N}^{-4}\ \mathrm{m}^{-4}$	10^{-6}
r		0.4

Table 3.1. Material parameters

Considering the above material parameters, the three eigenvalues in (3.2.56) are:

$$\begin{aligned} \lambda_1 &= 2.3324 \times 10^{-1}\ \mathrm{m}^2\ \mathrm{s}^{-1}, \\ \lambda_2 &= 4.0 \times 10^{-9}\ \mathrm{m}^2\ \mathrm{s}^{-1}, \\ \lambda_3 &= 1.8 \times 10^{-10}\ \mathrm{m}^2\ \mathrm{s}^{-1}. \end{aligned}$$

For the consolidation experiment, an inward force, $f_0 = 5$ MPa 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. All boundary conditions are described. Note that in this experiment, all the unknowns change immediately at $t = t_0$ s, thus another equilibrium will be established in the end. At the final equilibrium, the electro-chemical potentials $\tilde{\mu}^\beta$, $\beta = l, +, -$, have the same value as the value in the initial state. However, the stress and fluid pressure have changed, since the porous medium is compressed. Figure 3.3 displays the solutions. As it can be seen the time for consolidation to occur is approximately $t - t_0 \approx 0.16$ h.

For the free swelling experiment, the initial and boundary conditions are chosen. In this experiment, we decrease the external salt concentration with a small amount from $c_{out} = 1 \times 10^2$ mol m^{-3} to $c_{out} = 0.995 \times 10^2$ mol m^{-3}. Therefore, as on (3.2.42) $\tilde{\mu}^\beta$ changes accordingly. The displacement, pore pressure, electrical potential, electro-chemical potentials and ion concentrations are displayed in Figure 3.4.

The pore pressure increases from the initial value to the maximum value $p = 0.0041$ MPa at $t - t_0 \approx 0.09$ h.

3.2.4 Conclusions

The analytical solutions are derived for consolidation and free swelling experiments to verify the numerical finite element solutions. The governing equations are defined in Lagrangian coordinates. We assume an infinitesimal deformation for the solid skeleton and a sufficiently small change in the external salt concentration. By choosing ϵ from interval $10^{-5} \leq \epsilon \leq 10^{-15}$ the results do not change for both cases.

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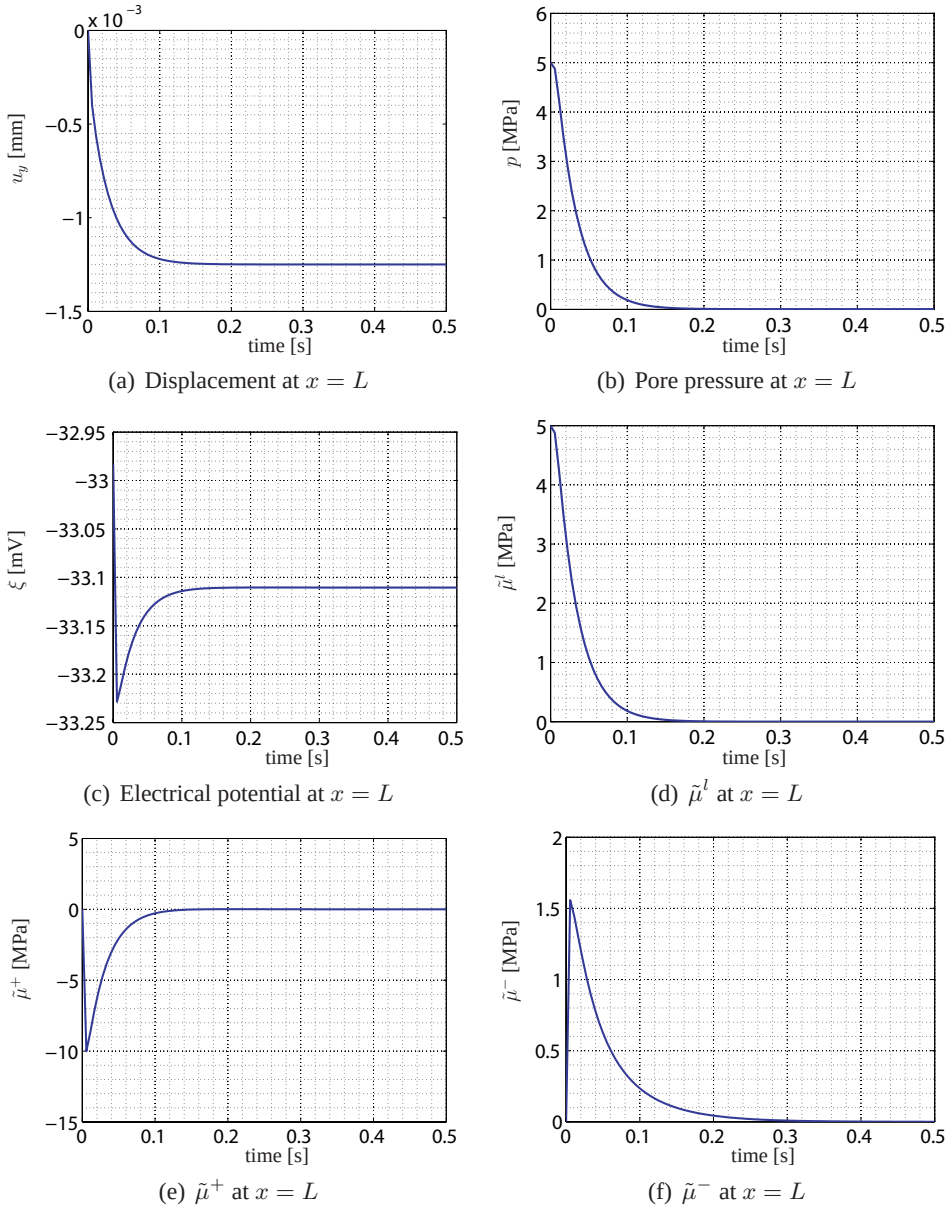
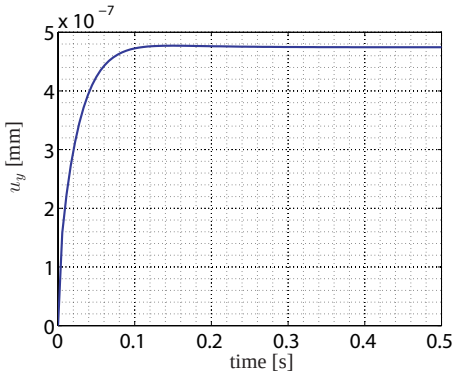


(a) Displacement at $x = L$ (b) Pore pressure at $x = L$

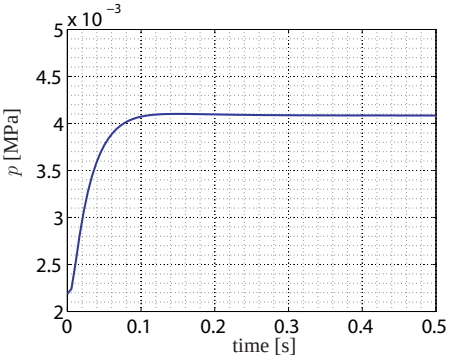
(c) Electrical potential at $x = L$ (d) $\tilde{\mu}^l$ at $x = L$

(e) $\tilde{\mu}^+$ at $x = L$ (f) $\tilde{\mu}^-$ at $x = L$

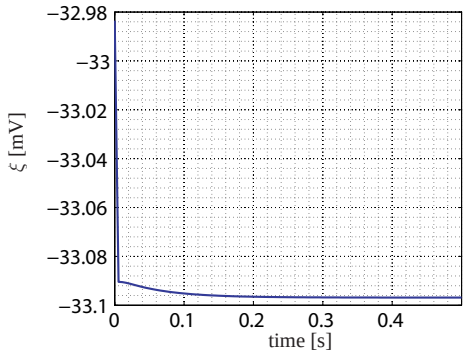
Figure 3.3. Results at $x = L$ for consolidation.



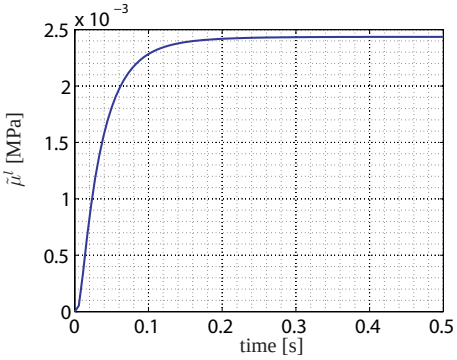
(a) Displacement at $x = L$



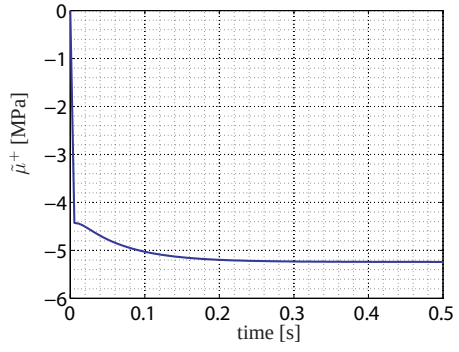
(b) Pore pressure at $x = L$



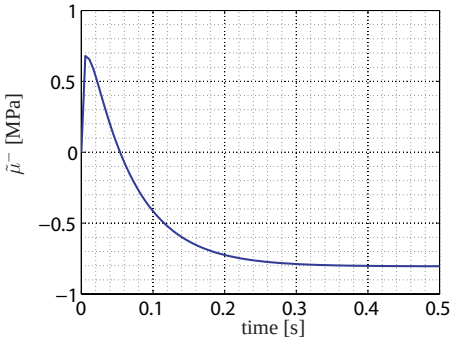
(c) Electrical potential at $x = L$



(d) $\tilde{\mu}^l$ at $x = L$



(e) $\tilde{\mu}^+$ at $x = L$



(f) $\tilde{\mu}^-$ at $x = L$

Figure 3.4. Results at $x = L$ for free swelling.

Chapter 4

Mixed and hybrid finite element solution for two-components

While searching for a quantitative description of physical phenomena, the engineer or physicist establishes generally a system of ordinary or partial differential equations valid in a certain region (or domain) and imposes on this system suitable boundary and initial conditions. At this stage the mathematical model is complete, and for practical applications "merely" a solution for a particular set of numerical data is needed. Here, however, come the major difficulties, as only the very simplest forms of equations, within geometrically trivial boundaries, are capable of being solved exactly with available mathematical methods.

To enlist the aid of the most powerful tool developed in this century - the digital computer - it is necessary to recast the problem in a purely algebraic form, involving only the basic arithmetic operations. To achieve this, various forms of discretisation of the continuum problem defined by differential equations can be used. In such a discretisation the infinite set of numbers representing the unknown function or functions is replaced by a finite number of unknown parameters, and this process, in general, requires some form of approximation.

Of the various forms of discretisation that are possible, one of the most used is the finite difference process. Another method that is often used in many physical applications is concerned with various trial function approximations falling under the general classification of finite element methods. It has been shown that even finite difference processes can be included as a subclass of this more general theory (Ciarlet, 1978).

The name "mixed method" is applied to a variety of finite element methods that have more than one approximation space. Typically one or more of the spaces play the role of Lagrange multipliers to enforce constraints. The name and many of the original concepts for such methods originated in solid mechanics where it was desirable to have a more accurate approximation of certain derivatives of displacement. However, for the Stokes equations that govern viscous fluid flow, the natural Galerkin approximation is a mixed method (Babuška, 1973), (Babuška and Aziz, 1973), (Brezzi, 1974), (Fortin, 1977) and (Brezzi and Fortin, 1991).

As it was mentioned, in a mixed formulation the gradient of the solution is introduced as a separate dependent variable of which the approximation is sought in a different finite element space than the solution itself.

The main advantage of this method is that it suffices to use finite elements of class C^0 whereas finite elements of class C^1 would be required for conforming methods. Another advantage (from the point of view of fluid mechanics and in particular our two- and four-component mixture model) is that the present method not only yields a continuous approximation of the solution, but also of the derivatives of the solution (which, in addition need to be computed).

The mixed finite element method has been extensively used for the solution of parabolic equations arising in different application fields. The mixed finite element method was proposed for two-dimensional problems by (Raviart and Thomas, 1977), (Thomas, 1977) and (Roberts and Thomas, 1991), and by Nédélec for three-dimensional problems (Nédélec, 1980) and (Nédélec, 1986).

Cartilaginous tissues are soft hydrated tissues with strong swelling and shrinkage properties. This swelling and shrinkage 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. In chapter 2 a finite deformation four-component model has been derived to account for osmotic effects. To account for finite deformation the set of equations is written in Lagrangian coordinates. This leads to a system of coupled time dependent non-linear equations together with boundary conditions.

In our model it is desirable to obtain approximations of the fluid flow and ions flow that fulfil the conservation equations. In finite element simulations (van Loon et al., 2003), these quantities are generally calculated by differentiation of the electrochemical potential solutions. This approach may lead to violation of the mass conservation principle.

The mixed finite element method provides an attractive framework for this type of problems by simultaneously approximating flows and electro chemical potentials. Flows computed by mixed finite elements automatically satisfy the "divergence free" property, both locally and globally, and the corresponding normal flux field is guaranteed to be continuous across inter-element boundaries. In this chapter the mixed finite element variational formulation is derived for the set of coupled equations describing the two-component model in general dimensions. Only the lowest-order mixed method will be considered, first, because higher order-methods result in some conceptual complications and, second, because the lowest-order method is comparatively easy and straightforward to use for practical problems.

It is more useful to propose the mixed method first for the linear two-component model (2.8.1). In fact this will give a basis from which to continue the mixed method for the four-component model.

This chapter is outlined as follows. In the first section preliminary definitions of function spaces are given. In section 2 we propose a mixed formulation for the two-component mixture. In this section the existence and uniqueness for the discretised system is proven. In section 3 we introduce the mixed hybrid technique. Section 4 is devoted to numerical results for given examples.

4.1 Notations and Preliminaries

In this section we will introduce some notations and definitions crucial for the mixed formulation (Ciarlet, 1978).

Throughout this article, Ω shall denote a bounded, open, connected subset of $\mathbb{R}^n$, $n = 1, 2, 3$, with a Lipschitz continuous boundary Γ (Ciarlet, 1978, p. 12).

Define $\Omega_T = \Omega \times (0, T]$ for $T > 0$ and consider the sets $\Gamma_{\mathbf{u}}^D$ and $\Gamma_{\mathbf{u}}^N$ (and similarly Γ_p^D and Γ_p^N) to be two disjoint open subsets of the total boundary $\Gamma = \partial\Omega$, such that

$$\Gamma_\alpha^D \cap \Gamma_\alpha^N = \emptyset \text{ and } \bar{\Gamma}_\alpha^D \cup \bar{\Gamma}_\alpha^N = \Gamma \text{ for } \alpha = \mathbf{u}, p.$$

We assume

$$\text{meas } \Gamma_\alpha^D > 0 \quad \text{for } \alpha = \mathbf{u}, p.$$

$L^2(\Omega)$ is the set of all Lebesgue measurable scalar functions $f : \Omega \to \mathbb{R}$ such that

$$\|f\|_0 = \left(\int_\Omega f^2 d\mathbf{x} \right)^{1/2} < \infty.$$

$\mathbf{L}^2(\Omega)$ is the set of all Lebesgue measurable vector functions $\mathbf{f} : \Omega \to \mathbb{R}^n$ such that

$$\|\mathbf{f}\|_0 = \left(\int_\Omega |\mathbf{f}|^2 d\mathbf{x} \right)^{1/2} < \infty.$$

Let k be a nonnegative integer, then $H^k(\Omega)$ denotes the Sobolev space,

$$H^k(\Omega) = \left\{ v \in L^2(\Omega) : \ D^\alpha v \in L^2(\Omega) \quad \text{for all } |\alpha| \le k \right\},$$

equipped with the norm

$$\|v\|_k = \sum_{|\alpha| \le k} \|D^\alpha v\|_0.$$

In the above definition

$$D^\alpha v = \frac{\partial^{|\alpha|} v}{\partial x_1^{\alpha_1} \cdots \partial x_n^{\alpha_n}}, \quad \alpha = (\alpha_1, \cdots, \alpha_n) \in \mathbb{N}^n \text{ with } |\alpha| = \sum_{i=1}^n \alpha_i,$$

where differentiation is to be understood in the weak sense.

Let $C_0^\infty(\Omega)$ denote the space of all infinitely differentiable scalar functions $\varphi : \Omega \to \mathbb{R}$ with compact support in Ω. We denote by $H_0^k(\Omega)$ the closure of the space $C_0^\infty(\Omega)$ in $H^k(\Omega)$. Moreover if we define

$$|v|_k = \sum_{|\alpha| = k} \|D^\alpha v\|_0.$$

Note that $|\cdot|_1$ and $\|\cdot\|_1$ are equivalent norms in $H_0^1(\Omega)$.

We denote by $H^{-k}(\Omega)$ the dual space to $H_0^k(\Omega)$. For $f \in H^{-k}(\Omega)$,

$$\|f\|_{-k} = \sup_{0 \neq v \in H_0^k(\Omega)} \frac{(f, v)}{\|v\|_k}$$

defines the related norm, where $(\cdot, \cdot)$ denotes the duality pairing between $H^{-k}(\Omega)$ and $H_0^k(\Omega)$.

Let $k = 1$, for $\varphi \in H^1(\Omega)$, the trace $\gamma_D \varphi = \varphi|_\Gamma$ is well-defined and is in $L^2(\Gamma)$. In other words there exists a constant C, depending only on Ω, such that

$$\|\varphi\|_{0,\Gamma} \leq C \|\varphi\|_1 \text{ for all } \varphi \in H^1(\Omega).$$

The image of the above trace mapping is denoted by

$$H^{1/2}(\Gamma) = \left\{ \gamma_D \varphi : \varphi \in H^1(\Omega) \right\},$$

and is a Hilbert space with norm

$$\|\psi\|_{1/2} = \inf_{\varphi \in H^1(\Omega)} \left\{ \|\varphi\|_1 : \psi = \gamma_D \varphi \right\}.$$

Define the functional space

$$H(\mathrm{div}; \Omega) = \{ \mathbf{q} \in \mathbf{L}^2(\Omega) : \ \nabla \cdot \mathbf{q} \in L^2(\Omega) \},$$

and the inner product

$$(\mathbf{q}_1, \mathbf{q}_2)_{\mathrm{div};\Omega} = \int_\Omega \left(\mathbf{q}_1 \cdot \mathbf{q}_2 + \nabla \cdot \mathbf{q}_1 \nabla \cdot \mathbf{q}_2 \right) \, d\mathbf{x} \quad \text{for all } \ \mathbf{q}_1, \mathbf{q}_2 \in H(\mathrm{div}; \Omega).$$

The space $H(\mathrm{div}; \Omega)$ with this inner product is a Hilbert space. The norm in $H(\mathrm{div}; \Omega)$ will be defined as

$$\|\mathbf{q}\|_{\mathrm{div};\Omega} = (\mathbf{q}, \mathbf{q})_{\mathrm{div};\Omega}^{1/2}.$$

If $\mathbf{q} \in H(\mathrm{div}; \Omega)$, then the trace $\gamma_N \mathbf{q} = \mathbf{n} \cdot \mathbf{q}$, where $\mathbf{n}$ is the outward normal to Γ, is well defined (Brezzi and Fortin, 1991, Lemma III.1.1) and we denote

$$H^{-1/2}(\Gamma) = \{ \gamma_N \mathbf{q} : \mathbf{q} \in H(\mathrm{div}; \Omega) \}$$

with norm

$$\|\mu\|_{-1/2,\Gamma} = \inf_{\mathbf{q} \in H(\mathrm{div};\Omega)} \{ \|\mathbf{q}\|_{H(\mathrm{div};\Omega)} : \mu = \gamma_N \mathbf{q} \text{ for all } \mu \in H^{-1/2}(\Gamma) \}.$$

We shall use the following version of Green's formula:

$$\int_\Omega (\varphi \nabla \cdot \mathbf{q} + \nabla \varphi \cdot \mathbf{q}) \, d\mathbf{x} = \int_\Gamma \varphi \mathbf{q} \cdot \mathbf{n} \, ds,$$

for all $\mathbf{q} \in H(\mathrm{div};\Omega)$ and $\varphi \in H^1(\Omega)$.

We also define the following linear spaces:

$$\begin{aligned}
\mathcal{V} &= \left\{\mathbf{u} \in (H^1(\Omega))^n : \mathbf{u} = 0 \text{ on } \Gamma_{\mathbf{u}}^D\right\} \\
H_D^1(\Omega) &= \left\{\varphi \in H^1(\Omega) : \varphi = 0 \text{ on } \Gamma_p^D\right\}, \\
H_D^{1/2}(\Gamma) &= \left\{\lambda \in H^{1/2}(\Gamma) : \lambda = 0 \text{ on } \Gamma_p^D\right\}, \\
H_N(\mathrm{div};\Omega) &= \left\{\mathbf{q} \in H(\mathrm{div};\Omega) : \mathbf{n}\cdot\mathbf{q} = 0 \text{ on } \Gamma_p^N\right\}, \\
H_N^{-1/2}(\Gamma) &= \left\{\mu \in H^{-1/2}(\Gamma) : \mu = 0 \text{ on } \Gamma_p^N\right\}.
\end{aligned}$$

4.2 A mixed variational formulation for the two-component model

Saturated porous media, such as saturated solids and sands, are modelled as a two-phase mixtures composed of deforming solid skeleton and saturated pore fluids. To numerically simulate the interaction of the fluid skeleton with the pore fluid, the media are modelled as porous continua, in which a representative element volume around any mathematical point in the medium is always assumed to contain the solid phase and porous fluid phase. Based on this, the two-component model is formulated in (2.8.1). In recent years, a lot of effort has been dedicated to the numerical treatment of this model. The numerical treatment of this model by the Taylor-Hood finite element was studied by (Murad and Loula, 1992) and (Murad and Loula, 1994). This work was continued with a detailed analytical investigation in (Murad and Thomée, 1996). A general reference for the use of the finite element method for the numerical simulation of fluid flow and deformation processes in porous media is the monograph (Lewis and Schrefler, 1998). Our purpose in this section is to study the mixed method for the coupled flow problem (2.8.1):

		Conservation Equations	
$\mathbf{0}$	$=$	$\nabla\cdot\boldsymbol{\sigma} - \nabla p,$	
0	$=$	$\dfrac{\partial \nabla\cdot\mathbf{u}}{\partial t} + \nabla\cdot\mathbf{q},$	
		Constitutive Equations	
$\boldsymbol{\sigma}$	$=$	$2\mu_s\boldsymbol{\mathcal{E}} + \lambda_s \mathrm{tr}\boldsymbol{\mathcal{E}}, \quad \boldsymbol{\mathcal{E}} = \dfrac{1}{2}(\nabla\mathbf{u} + (\nabla\mathbf{u}^T)),$	
$\mathbf{q}$	$=$	$-K\nabla p,$	
		Secondary Equation	
φ	$=$	$1 - (1-\varphi_0)(1-\nabla\cdot\mathbf{u})$	
		Boundary Conditions	
$\mathbf{u}$	$=$	$\mathbf{0}$	on $\Gamma_{\mathbf{u}}^D \times (0,T]$,
p	$=$	0	on $\Gamma_p^D \times (0,T]$,
$\mathbf{g}_{\mathbf{u}}^N$	$=$	$\mathbf{n}\cdot(\boldsymbol{\sigma}(\mathbf{u}) - p)$	on $\Gamma_{\mathbf{u}}^N \times (0,T]$,
$\mathbf{n}\cdot\mathbf{q}$	$=$	0	on $\Gamma_p^N \times (0,T]$,

where, we omitted the superscript l from $\mathbf{q}^l$ in (2.8.1).

4.2.1 Variational formulation

For the preliminary step of defining a spatially semi-discrete approximate solution to our initial boundary value problem, we write the problem in weak form. Considering the flux $\mathbf{q}$ and the flux space $H_N(\mathrm{div};\Omega)$, the above system of equations can be formally written as a first- order system whose mixed variational formulation gives rise to the following system of variational equations:
Find $(\mathbf{u},\mathbf{q},p)(\cdot,t) \in \mathcal{V} \times H_N(\mathrm{div};\Omega) \times L^2(\Omega)$, such that

$$\begin{cases} \displaystyle\int_\Omega \left(2\mu_s \boldsymbol{\mathcal{E}}(\mathbf{u}) : \boldsymbol{\mathcal{E}}(\bar{\mathbf{u}}) + \lambda_s \nabla\cdot\mathbf{u}\nabla\cdot\bar{\mathbf{u}}\right) d\mathbf{x} - \int_\Omega p\nabla\cdot\bar{\mathbf{u}}\, d\mathbf{x} = \int_{\Gamma_{\mathbf{u}}^N} \mathbf{g}_{\mathbf{u}}^N \cdot \bar{\mathbf{u}}\, ds, & \text{(4.2.1a)} \\ \displaystyle\frac{1}{K}\int_\Omega \mathbf{q}\cdot\bar{\mathbf{q}}\, d\mathbf{x} - \int_\Omega p\nabla\cdot\bar{\mathbf{q}}\, d\mathbf{x} = 0, & \text{(4.2.1b)} \\ \displaystyle -\int_\Omega \nabla\cdot\mathbf{q}\bar{p}\, d\mathbf{x} - \int_\Omega \frac{\partial\nabla\cdot\mathbf{u}}{\partial t}\bar{p}\, d\mathbf{x} = 0, & \text{(4.2.1c)} \end{cases}$$

for all test functions $(\bar{\mathbf{u}},\bar{\mathbf{q}},\bar{p}) \in \mathcal{V} \times H_N(\mathrm{div};\Omega) \times L^2(\Omega)$ and $t > 0$. Note that the solution is time-dependent.

Define

$$\begin{aligned} a(\mathbf{u},\bar{\mathbf{u}}) &= \int_\Omega \left(2\mu_s \boldsymbol{\mathcal{E}}(\mathbf{u}) : \boldsymbol{\mathcal{E}}(\bar{\mathbf{u}}) + \lambda_s \nabla\cdot\mathbf{u}\nabla\cdot\bar{\mathbf{u}}\right) d\mathbf{x}, \\ b(\mathbf{u},\bar{p}) &= -\int_\Omega \nabla\cdot\mathbf{u}\bar{p}\, d\mathbf{x}, \\ c(\mathbf{q},\bar{\mathbf{q}}) &= \frac{1}{K}\int_\Omega \mathbf{q}\cdot\bar{\mathbf{q}}\, d\mathbf{x}, \\ d(\bar{\mathbf{q}},p) &= -\int_\Omega \nabla\cdot\bar{\mathbf{q}}p\, d\mathbf{x}, \\ f(\bar{\mathbf{u}}) &= \int_{\Gamma_{\mathbf{u}}^N} \mathbf{g}_{\mathbf{u}}^N \cdot \bar{\mathbf{u}}\, ds, \end{aligned}$$

then the problem (4.2.1a)-(4.2.1c) can be rewritten as follows:

Find $(\mathbf{u},\mathbf{q},p) \in \mathcal{V} \times H_N(\mathrm{div};\Omega) \times L^2(\Omega)$ such that

$$\begin{aligned} a(\mathbf{u},\bar{\mathbf{u}}) \quad\quad + b(\bar{\mathbf{u}},p) &= f(\bar{\mathbf{u}}), \\ c(\mathbf{q},\bar{\mathbf{q}}) + d(\bar{\mathbf{q}},p) &= 0, \\ \frac{d}{dt}b(\mathbf{u},\bar{p}) + d(\mathbf{q},\bar{p}) &= 0, \end{aligned} \qquad (4.2.2)$$

for all test functions $(\bar{\mathbf{u}}, \bar{\mathbf{q}}, \bar{p}) \in \mathcal{V} \times H_N(\mathrm{div}; \Omega) \times L^2(\Omega)$ and $t > 0$.

We shall use the implicit Euler scheme for time discretisation. Let Δt be the time step and $(\mathbf{u}_n, \mathbf{q}_n, p_n)$ the approximation of the solution vector $(\mathbf{u}, \mathbf{q}, p)$ at $t = t_n = n\Delta t$. Then the system of equations (4.2.2) resulting from backward Euler is:

$$\boxed{\begin{array}{l}\text{Find } (\mathbf{u}_n, \mathbf{q}_n, p_n) \in \mathcal{V} \times H_N(\mathrm{div}; \Omega) \times L^2(\Omega) \text{ such that} \\ \\ \begin{array}{lll} a(\mathbf{u}_n, \bar{\mathbf{u}}) & +b(\bar{\mathbf{u}}, p_n) & = \quad f(\bar{\mathbf{u}}), \\ \Delta t c(\mathbf{q}_n, \bar{\mathbf{q}}) & +\Delta t d(\bar{\mathbf{q}}, p_n) & = \quad 0, \\ b(\mathbf{u}_n, \bar{p}) & +\Delta t d(\mathbf{q}_n, \bar{p}) & = b(\mathbf{u}_{n-1}, \bar{p}), \end{array}\end{array}} \tag{4.2.3}$$

for all test functions $(\bar{\mathbf{u}}, \bar{\mathbf{q}}, \bar{p}) \in \mathcal{V} \times H_N(\mathrm{div}; \Omega) \times L^2(\Omega)$.

Define two new bilinear forms

$$\mathbb{A}(\mathbf{u}, \mathbf{q}; \bar{\mathbf{u}}, \bar{\mathbf{q}}) = a(\mathbf{u}, \bar{\mathbf{u}}) + \Delta t c(\mathbf{q}, \bar{\mathbf{q}}), \tag{4.2.4}$$

$$\mathbb{B}(\mathbf{u}, \mathbf{q}; \bar{p}) = b(\mathbf{u}, \bar{p}) + \Delta t d(\mathbf{q}, \bar{p}), \tag{4.2.5}$$

and the linear forms

$$\begin{aligned} F(\bar{\mathbf{u}}) &= (0, f(\bar{\mathbf{u}}))^T, \\ G_n(\bar{p}) &= b(\mathbf{u}_{n-1}, \bar{p}), \end{aligned}$$

then (4.2.3) is rewritten as

$$\boxed{\begin{array}{l}\text{Find } (\mathbf{u}_n, \mathbf{q}_n, p_n) \in \mathcal{V} \times H_N(\mathrm{div}; \Omega) \times L^2(\Omega) \text{ such that} \\ \\ \begin{array}{ll} \mathbb{A}(\mathbf{u}_n, \mathbf{q}_n; \bar{\mathbf{u}}, \bar{\mathbf{q}}) + \mathbb{B}(\bar{\mathbf{u}}, \bar{\mathbf{q}}; p_n) & = F(\bar{\mathbf{u}}), \\ \mathbb{B}(\mathbf{u}_n, \mathbf{q}_n; \bar{p}) & = G(\bar{p}), \end{array}\end{array}} \tag{4.2.6}$$

for all test functions $(\bar{\mathbf{u}}, \bar{\mathbf{q}}, \bar{p}) \in \mathcal{V} \times H_N(\mathrm{div}; \Omega) \times L^2(\Omega)$. Note that

$$g_n(\bar{p}) = \mathbb{B}(\mathbf{u}_{n-1}, \mathbf{0}; \bar{p}).$$

Hereafter, we shall study the numerical methods for solving (4.2.6). In order to simplify the notation, we shall omit the subscript n in the sequel.

4.2.2 Existence and uniqueness

The above problem is a saddle point problem. For the existence and uniqueness of the solution for (4.2.6) we abstract the key futures of a general saddle point problem. This analysis can be found in (Brezzi and Fortin, 1991, Section II.1), although the exposition in (Brenner and Scott, 1994, Section 11.2) is more comprehensive and we will mainly follow the later analysis.

Let V and Q be Hilbert spaces with inner products $(\cdot, \cdot)_V$, $(\cdot, \cdot)_Q$ and associated norms $\|\cdot\|_V$, $\|\cdot\|_Q$, respectively. Define two bilinear forms

$$\begin{aligned} a(\cdot, \cdot) &: V \times V \to \mathbb{R}, \\ b(\cdot, \cdot) &: V \times Q \to \mathbb{R}. \end{aligned}$$

It is natural to assume that these forms are continuous:

$$\begin{array}{rcll} a(u,v) & \leq & \|a\|\|u\|_V\|v\|_V & \text{for all } u,v \in V, \\ b(u,p) & \leq & \|b\|\|u\|_V\|p\|_Q & \text{for all } u \in V, p \in Q. \end{array}$$

We denote by V^* and Q^* the dual spaces of V and Q, respectively and further suppose that bounded linear functionals $f \in V^*$ and $g \in Q^*$ are given. We investigate the existence and uniqueness of a solution of the saddle point problem:

$$\boxed{\begin{array}{l} \text{Find } (u,p) \in V \times Q \text{ such that} \\ \\ \begin{array}{lll} a(u,v) + b(v,p) & = (f,v)_{V^*,V}\,, & v \in V, \\ b(u,q) & = (g,q)_{Q^*,Q}\,, & q \in Q. \end{array} \end{array}} \tag{4.2.7}$$

Denote by $A : V \to V^*$ and $B : V \to Q^*$ the bounded linear operators associated with the bilinear forms $a(\cdot,\cdot)$ and $b(\cdot,\cdot)$ according to

$$\begin{array}{rcll} (Au,v)_{V^*,V} & = & a(u,v), & u,v \in V, \\ (Bv,q)_{Q^*,Q} & = & b(v,q), & v \in V, q \in Q, \end{array}$$

and

$$\begin{array}{rcl} F(v) & = & (f,v)_{V^*,V}, \\ G(q) & = & (g,q)_{Q^*,Q}, \end{array}$$

then the saddle point (4.2.7) can be equivalently written as the following system of operator equations

$$\begin{array}{rcrcl} Au & + & B^*p & = & F \text{ in } V^*, \\ Bu & & & = & G \text{ in } Q^*. \end{array}\,, \tag{4.2.8}$$

The kernels of the operator B and B^* are defined by

$$\begin{array}{rcl} \ker(B) & = & \{u \in V \mid b(u,q) = 0 \text{ for all } q \in Q\}, \\ \ker(B^*) & = & \{q \in Q \mid b(u,q) = 0 \text{ for all } u \in V\}, \end{array}$$

Theorem 4.1 (Existence and uniqueness result)**.** *Let V and Q be Hilbert spaces and let $a(\cdot,\cdot) : V \times V \to \mathbb{R}$ and $b(\cdot,\cdot) : V \times Q \to \mathbb{R}$ be bounded bilinear forms with associated operators $A : V \to V^*$ and $B : V \to Q^*$ such that there holds:*

(i) The bilinear form $a(\cdot,\cdot)$ is $\ker(B)$-elliptic, i.e., there exists a constant $\alpha > 0$ such that

$$a(v_0,v_0) \geq \alpha \|v_0\|_V^2, \quad v_0 \in \ker(B).$$

(ii) The bilinear $b(\cdot,\cdot)$ satisfies the inf-sup condition

$$\inf_{q \in Q \setminus \ker(B^*)} \sup_{v \in V} \frac{b(v,q)}{\|v\|_V \|q\|_{Q \setminus \ker(B^*)}} \geq \beta.$$

Then for any $f \in V^*$ and $g \in \mathrm{Im}(B)$, the saddle point problem (4.2.7) *admits a solution $(u,p) \in V \times Q$, where $u \in V$ is uniquely determined and $p \in Q$ is unique up to an element of $\ker(B^*)$. Moreover one has the bounds*

$$\|u\|_V \leq \frac{1}{\alpha}\|f\|_{V^*} + \left(1 + \frac{\|a\|}{\alpha}\right)\frac{1}{\beta}\|g\|_{Q^*}, \tag{4.2.9}$$

$$\|p\|_{Q\backslash\ker(B^*)} \leq \frac{1}{\beta}\left(1 + \frac{\|a\|}{\alpha}\right)\|f\|_{V^*} + \frac{\|a\|}{\beta^2}\left(1 + \frac{\|a\|}{\alpha}\right)\|g\|_{Q^*}. \tag{4.2.10}$$

Proof. See for example (Brezzi and Fortin, 1991, Chapter 2). ■

Now we return to the saddle point problem (4.2.6). We equip the space $\mathcal{V} \times H_N(\mathrm{div};\Omega)$ with a norm

$$|||\,(\mathbf{u},\mathbf{q})|||_1 = \left(\|\mathbf{u}\|_1^2 + \|\mathbf{q}\|_{\mathrm{div};\Omega}^2\right)^{1/2}. \tag{4.2.11}$$

To prove the $\ker(\mathbb{B})$-ellipticity of $\mathbb{A}$, we need the following lemma.

Lemma 4.2 (Korn's second inequality)**.** *Let $\Omega \subset \mathbb{R}^3$ be an open bounded set with smooth boundary. In addition, suppose that $\Gamma_0 \subset \partial\Omega$ has positive two-dimensional measure. Then there exists a positive number $c(\Omega,\Gamma_0)$ such that*

$$\int_\Omega \boldsymbol{\mathcal{E}}(\mathbf{u}) : \boldsymbol{\mathcal{E}}(\mathbf{u})\, d\mathbf{x} \geq c(\Omega,\Gamma_0)\|\mathbf{u}\|_1^2 \quad \textit{for all } \mathbf{u} \in \mathcal{V}. \tag{4.2.12}$$

Proof. See for example (Brezzi and Fortin, 1991). ■

Using Korn's inequality, we show that the bilinear form $\mathbb{A}$ is $\ker(\mathbb{B})$-elliptic on $\mathcal{V} \times H_N(\mathrm{div};\Omega)$. The definition of the subspace $\ker(\mathbb{B})$ implies that

$$\nabla\cdot\mathbf{u} + \Delta t\nabla\cdot\mathbf{q} = 0 \quad \text{for all } (\mathbf{u},\mathbf{q}) \in \ker(\mathbb{B}). \tag{4.2.13}$$

Using Korn's inequality, we get

$$\begin{aligned}
\mathbb{A}((\mathbf{u},\mathbf{q}),(\mathbf{u},\mathbf{q})) &= a(\mathbf{u},\bar{\mathbf{u}}) + \Delta t c(\mathbf{q},\bar{\mathbf{q}}) \\
&\geq 2\mu_s c\|\mathbf{u}\|_1^2 + \lambda_s\|\nabla\cdot\mathbf{u}\|_0^2 + K^{-1}\Delta t\|\mathbf{q}\|_0^2 \\
&= 2\mu_s c\|\mathbf{u}\|_1^2 + \lambda_s(\Delta t)^2\|\nabla\cdot\mathbf{q}\|_0^2 + K^{-1}\Delta t\|\mathbf{q}\|_0^2 \\
&\geq \alpha\left(\|\mathbf{u}\|_1^2 + \|\mathbf{q}\|_{\mathrm{div};\Omega}^2\right) \\
&= \alpha\,|||\,(\mathbf{u},\mathbf{q})|||_1^2,
\end{aligned} \tag{4.2.14}$$

for all $(\mathbf{u},\mathbf{q}) \in \ker(\mathbb{B})$ and where $\alpha = \min(2\mu_s c, \lambda_s(\Delta t)^2, K^{-1}\Delta t)$.

The second condition in Theorem 4.1 is inf-sup condition:

$$\sup_{(\mathbf{u},\mathbf{q})\in\mathcal{V}\times H_N(\mathrm{div};\Omega)} \frac{\mathbb{B}(q,(\mathbf{u},\mathbf{q}))}{|||(\mathbf{u},\mathbf{q})|||_1} \geq \beta\|q\|, \quad \text{for all } q \in L^2(\Omega), \tag{4.2.15}$$

where we assume implicitly that the left side has to be evaluated only for $\|(\mathbf{u},\mathbf{q})\|_1 \neq 0$. We restrict the supremum to a subset of functions $(\mathbf{0},\mathbf{q})$, therefore we obtain a lower estimate for β:

$$\Delta t \sup_{\mathbf{q}\in H_N(\mathrm{div};\Omega)} \frac{d(q,\mathbf{q})}{\|\mathbf{q}\|_{\mathrm{div};\Omega}} \geq \tilde{\beta}\|q\|_0, \quad \text{for all } q \in L^2(\Omega). \tag{4.2.16}$$

We need the following lemma to prove this inequality:

Lemma 4.3. *There exists a positive constant C such that for all $q \in L^2(\Omega)$ there exists a function $\tilde{\mathbf{q}} \in H_N(\mathrm{div};\Omega)$ satisfying*

$$-\nabla\cdot\tilde{\mathbf{q}} = q$$

and

$$\|\tilde{\mathbf{q}}\|_{\mathrm{div};\Omega} \leq C\|q\|_0.$$

Proof. Let $q \in L^2(\Omega)$, then by the Lax-Miligram Theorem (Brenner and Scott, 1994, Theorem 2.7.7) there exists a unique $\Phi \in H^1_D(\Omega)$ satisfying

$$\begin{cases} -\Delta\Phi &= q \quad \text{in } \Omega, \\ \nabla\Phi\cdot\mathbf{n} &= 0 \quad \text{on } \Gamma_p^N. \end{cases}$$

If we define $\tilde{\mathbf{q}} = \nabla\Phi$, then $\tilde{\mathbf{q}} \in H_N(\mathrm{div};\Omega)$ and we have

$$\int_\Omega \tilde{\mathbf{q}}\nabla\bar{\Phi}d\mathbf{x} = \int_\Omega q\bar{\Phi}d\mathbf{x} \quad \text{for all } \bar{\Phi} \in H^1_D(\Omega).$$

By choosing $\bar{\Phi} = \Phi$, we have

$$\|\tilde{\mathbf{q}}\|_0^2 = \int_\Omega q\Phi\, d\mathbf{x} \leq \|q\|_0\|\Phi\|_0 \leq C(\Omega)\|q\|_0\|\nabla\Phi\|_0,$$

where the last inequality was derived by the Poincaré inequality (Brenner and Scott, 1994, Proposition 5.3.5). ∎

Let $q \in L^2(\Omega)$, then by above the lemma there exists a function $\tilde{\mathbf{q}} \in H_N(\mathrm{div};\Omega)$ such that $-\nabla\cdot\tilde{\mathbf{q}} = q$ and

$$\|\tilde{\mathbf{q}}\|_{\mathrm{div};\Omega} \leq C\|q\|_0$$

for some constant C. Use the fact that

$$d(\tilde{\mathbf{q}},q) = -\int_\Omega \nabla\cdot\tilde{\mathbf{q}}q\, d\mathbf{x} = \int_\Omega q^2\, d\mathbf{x} = \|q\|_0^2,$$

thus

$$\Delta t \sup_{\mathbf{q}\in H_N(\mathrm{div};\Omega)} \frac{d(q,\mathbf{q})}{\|\mathbf{q}\|_{\mathrm{div};\Omega}} \geq \Delta t \frac{d(q,\tilde{\mathbf{q}})}{\|\tilde{\mathbf{q}}\|_{\mathrm{div};\Omega}} \geq \frac{\Delta t}{C}\|q\|_0.$$

Therefore the inf-sup condition holds for all $\beta \leq \dfrac{\Delta t}{C}$. The following result follows immediately from Theorem 4.1.

Theorem 4.4. *The saddle point problem* (4.2.6)*:*

$$\boxed{\begin{array}{l}\text{Find } (\mathbf{u},\mathbf{q},p)\in\mathcal{V}\times H_N(\mathrm{div};\Omega)\times L^2(\Omega) \text{ such that}\\ \\ \begin{array}{ll}\mathbb{A}(\mathbf{u},\mathbf{q};\bar{\mathbf{u}},\bar{\mathbf{q}})+\mathbb{B}(\bar{\mathbf{u}},\bar{\mathbf{q}};p) & =F(\bar{\mathbf{u}}),\\ \mathbb{B}(\mathbf{u},\mathbf{q};\bar{p}) & =G(\bar{p}),\end{array}\end{array}}$$

has a unique solution. moreover one has the bounds

$$|||\,(\mathbf{u}_n,\mathbf{q}_n)|||_1\le\frac{1}{\alpha}\|F\|_{-1}+\left(1+\frac{\|\mathbb{A}\|}{\alpha}\right)\frac{1}{\beta}\|\mathbb{B}\|\|\mathbf{u}_{n-1}\|_1, \tag{4.2.17}$$

$$\|p_n\|_{L^2(\Omega)\backslash\ker(\mathbb{B}^*)}\le\frac{1}{\beta}\left(1+\frac{\|\mathbb{A}\|}{\alpha}\right)\|F\|_{-1}+\frac{\|\mathbb{A}\|}{\beta^2}\left(1+\frac{\|\mathbb{A}\|}{\alpha}\right)\|\mathbb{B}\|\|\mathbf{u}_{n-1}\|_1. \tag{4.2.18}$$

4.2.3 Mixed finite element approximation

Assume that Ω is a polygon (n=2) or a polyhedron (n=3). We denote by $\mathcal{T}_h$ a triangulation of $\overline{\Omega}$ by n-simplices T of diameter not greater than h (T is a triangle or rectangle for $n=2$, a tetrahedron or block for $n=3$), where

$$\overline{\Omega}=\bigcup_{T\in\mathcal{T}_h}T.$$

For the definition of a triangulation, see (Ciarlet, 1978, page 38), for example. We shall also use the notation:

- meas T = the Euclidian measure of T in $\mathbb{R}^n$ (geometric area if $n=2$, geometric volume if $n=3$),
- h_T = the diameter of T, which in case of a triangulation by simplices, is just the length of the longest edge,
- ρ_T = the radius of the circle inscribed in T if $n=2$, or of the sphere inscribed in T if $n=3$,
- $h=\max\limits_{T\in\mathcal{T}_h}h_T$.

A family of triangulations $\{\mathcal{T}_h : h>0\}$ is said to be regular if

$$\inf_{h>0}h=0,\qquad \inf_{h>0}\min_{T\in\mathcal{T}_h}\frac{\rho_T}{h_T}>0.$$

Now in order to state a finite element formulation of problem (4.2.6), it is necessary to define finite-dimensional subspaces of $\mathcal{V}$, $H_N(\mathrm{div};\Omega)$ and $L^2(\Omega)$.

Let $H(\mathrm{div};\mathcal{T}_h)$ be the space of square-integrable vectorial functions $\mathbf{q}\in\mathbf{L}^2(\Omega)$, whose divergences are square -integrable on every sub-domain $T\in\mathcal{T}_h$, i.e.

$$H(\mathrm{div};\mathcal{T}_h)=\{\mathbf{q}\in\mathbf{L}^2(\Omega):\ \mathbf{q}|_T\in H(\mathrm{div};T)\ \text{ for all } T\in\mathcal{T}_h\},\tag{4.2.19}$$

with norm

$$\|\mathbf{q}\|_{\mathrm{div};\mathcal{T}_h}=\left(\|\mathbf{q}\|_0^2+\sum_{T\in\mathcal{T}_h}\|\nabla\cdot\mathbf{q}|_T\|_0^2\right)^{1/2}.\tag{4.2.20}$$

The following lemma gives a characterization of the functions in $H_N(\mathrm{div};\Omega)$.

Lemma 4.5. *A function $\mathbf{q}\in H(\mathrm{div};\mathcal{T}_h)$ is in $H_N(\mathrm{div};\Omega)$, if and only if*

$$\sum_{T\in\mathcal{T}_h}\int_{\partial T}\Phi\mathbf{n}_T\cdot\mathbf{q}\,ds=0\quad \textit{for all } \Phi\in H_D^1(\Omega).$$

Proof. ($\Rightarrow$) Let $\mathbf{q}\in H(\mathrm{div};\mathcal{T}_h)$ and suppose that the above inequality holds. Define $f\in L^2(\Omega)$ by

$$f|_T=\nabla\cdot\mathbf{q}|_T\quad\text{for all } T\in\mathcal{T}_h,$$

then

$$\begin{aligned}\int_\Omega f\Phi\,d\mathbf{x} &= \sum_{T\in\mathcal{T}_h}\int_T\nabla\cdot\mathbf{q}|_T\Phi\,d\mathbf{x}\\ &= \sum_{T\in\mathcal{T}_h}\int_{\partial T}\Phi\mathbf{n}_T\cdot\mathbf{q}\,ds-\sum_{T\in\mathcal{T}_h}\int_T\mathbf{q}\cdot\nabla\Phi\,d\mathbf{x}\\ &= -\sum_{T\in\mathcal{T}_h}\int_{\partial T}\mathbf{q}\cdot\nabla\Phi\,d\mathbf{x}\\ &= -\int_\Omega\mathbf{q}\cdot\nabla\Phi\,d\mathbf{x}\quad\text{for all }\ \Phi\in C_0^\infty(\Omega).\end{aligned}$$

Therefore $f=\nabla\cdot\mathbf{q}$ and thus $\mathbf{q}\in H(\mathrm{div};\Omega)$. Finally Green's formula implies

$$\int_\Gamma\Phi\mathbf{n}\cdot\mathbf{q}\,ds=\sum_{T\in\mathcal{T}_h}\int_{\partial T}\Phi\mathbf{n}_T\cdot\mathbf{q}\,ds=0\quad\text{for all }\ \Phi\in H_D^1(\Omega),$$

thus $\mathbf{n}\cdot\mathbf{q}=0$ on Γ_N^p. Therefore $\mathbf{q}\in H_N(\mathrm{div};\Omega)$.
($\Leftarrow$) Let $\mathbf{q}\in H_N(\mathrm{div};\Omega)$, then $\mathbf{q}\in H_N(\mathrm{div};\mathcal{T}_h)$ and

$$\sum_{T\mathcal{T}_h}\int_{\partial T}\Phi\mathbf{n}_T\cdot\mathbf{q}\,ds=\int_\Gamma\Phi\mathbf{n}\cdot\mathbf{q}\,ds=0\quad\text{for all }\ \Phi\in H_D^1(\Omega).$$

■

The following lemma gives an abstract view for the approximation of the problem (4.2.6). It provides the conditions for the existence and uniqueness of the approximated solution.

Lemma 4.6. *Let $\mathcal{V}_h \subset \mathcal{V}$, $\mathcal{W}_h \subset H_N(\mathrm{div};\Omega)$ and $\mathcal{Q}_h \subset L^2(\Omega)$ be finite dimensional subspaces. Denote by*

$$\begin{aligned} \mathbb{A}_h : \mathcal{V}_h \times \mathcal{W}_h &\rightarrow \mathcal{V}_h \times \mathcal{W}_h, \\ \mathbb{B}_h : \mathcal{V}_h \times \mathcal{W}_h &\rightarrow \mathcal{Q}_h, \end{aligned}$$

the bounded linear operators associated with the bilinear form $\mathbb{A}$ and $\mathbb{B}$ restricted to the finite dimensional subspaces $\mathcal{V}_h \times \mathcal{W}_h$ and $\mathcal{Q}_h$. Consider the following problem:

Find $(\mathbf{u}_h, \mathbf{q}_h, p_h) \in \mathcal{V}_h \times \mathcal{W}_h \times \mathcal{Q}_h$ such that

$$\begin{aligned} \mathbb{A}(\mathbf{u}_h, \mathbf{q}_h; \bar{\mathbf{u}}_h, \bar{\mathbf{q}}_h) + \mathbb{B}(\bar{\mathbf{u}}_h, \bar{\mathbf{q}}_h; p_h) &= f(\bar{\mathbf{u}}_h), \\ \mathbb{B}(\mathbf{u}_h, \mathbf{q}_h; \bar{p}_h) &= g(\bar{p}_h), \end{aligned}$$

for all test functions $(\bar{\mathbf{u}}_h, \bar{\mathbf{q}}_h, \bar{p}_h) \in \mathcal{V}_h \times \mathcal{W}_h \times \mathcal{Q}_h$.
In the same way as for the continuous problem, we define a closed subspace of $\mathcal{V}_h \times \mathcal{W}_h$:

$$\ker(\mathbb{B}_h) = \{(\mathbf{u}_h, \mathbf{q}_h) \in \mathcal{V}_h \times \mathcal{W}_h : \mathbb{B}(\mathbf{u}_h, \mathbf{q}_h; q_h) = 0 \text{ for all } q_h \in \mathcal{Q}_h\}.$$

If $\mathrm{div}\, \mathcal{V}_h + \mathrm{div}\, \mathcal{W}_h = \mathcal{Q}_h$, then

1. $\ker(\mathbb{B}_h) \subset \ker(\mathbb{B})$,
2. *$\mathbb{A}$ is $\ker(B_h)$-elliptic, i.e., there exists an $\alpha > 0$ such that*

$$\mathbb{A}_h(\mathbf{u}_h, \mathbf{q}_h; \mathbf{u}_h, \mathbf{q}_h) \geq \alpha \,|||\, (\mathbf{u}_h, \mathbf{q}_h) \,|||_1^2 \quad \text{for all } (\mathbf{u}_h, \mathbf{q}_h) \in \ker(\mathbb{B}_h),$$

3. *$\mathbb{B}$ satisfies the LBB condition, i.e., there exists a $\beta > 0$ such that*

$$\sup_{(\mathbf{u}_h, \mathbf{q}_h) \in \mathcal{V}_h \times \mathcal{W}_h} \frac{\mathbb{B}(\mathbf{u}_h, \mathbf{q}_h; q_h)}{|||(\mathbf{u}_h, \mathbf{q}_h)|||_1} \geq \beta \|q_h\| \quad \text{for all } q_h \in \mathcal{Q}_h,$$

Proof. See (Brezzi and Fortin, 1991, p.138) ■

Existence and uniqueness of the solution $(\mathbf{u}_h, \mathbf{q}_h, p_h) \in \mathcal{V}_h \times \mathcal{W}_h \times \mathcal{Q}_h$ follows, as in the continuous problem, directly from Theorem 4.1. Additionally, we can derive error estimates in the terms of approximation properties of the spaces $\mathcal{V}_h$, $\mathcal{W}_h$ and $\mathcal{Q}_h$.

Theorem 4.7. *If $\mathrm{div}\, \mathcal{V}_h + \mathrm{div}\, \mathcal{W}_h = \mathcal{Q}_h$, then the mentioned saddle point problem in the above lemma has a unique solution $(\mathbf{u}_h, \mathbf{q}_h, p_h) \in \mathcal{V}_h \times \mathcal{W}_h \times \mathcal{Q}_h$. Moreover,*

if $(\mathbf{u}, \mathbf{q}, p) \in \mathcal{V} \times H_N(\mathrm{div}; \Omega) \times L^2(\Omega)$ *is the solution of problem* (4.2.6)*, then we have the following estimates:*

$$\begin{aligned} |||(\mathbf{u}, \mathbf{q}) - (\mathbf{u}_h, \mathbf{q}_h)|||_1 &\leq C \inf_{(\tilde{\mathbf{u}}, \tilde{\mathbf{q}}) \in \mathcal{V}_h \times \mathcal{W}_h} |||(\mathbf{u}, \mathbf{q}) - (\tilde{\mathbf{u}}, \tilde{\mathbf{q}})|||_1, \\ \|p - p_h\|_{L^2(\Omega)} &\leq C \left(\inf_{\tilde{p} \in \mathcal{W}_h} \|p - \tilde{p}\|_0 + \inf_{(\tilde{\mathbf{u}}, \tilde{\mathbf{q}}) \in \mathcal{V}_h \times \mathcal{W}_h} |||(\mathbf{u}, \mathbf{q}) - (\tilde{\mathbf{u}}, \tilde{\mathbf{q}})|||_1 \right), \end{aligned}$$

where C *is a generic constant that depends on* α*,* β*,* $\|\mathbb{A}\|$ *and* $\|\mathbb{B}\|$*.*

Proof. See (Brezzi and Fortin, 1991, proposition II.2.6-7). ■

4.2.4 Raviart-Thomas-Nédélec elements

Remember the given triangulation $\mathcal{T}_h$ for Ω. Take $T \in \mathcal{T}_h$ and let $k \geq 0$ be an integer. Define

$$P^k(T): \quad \text{the space of polynomials of degree } \leq k.$$

the dimension of $P^k(T)$ is $\frac{1}{2}(k+1)(k+2)$ and $\frac{1}{6}(k+1)(k+2)(k+3)$ for $n = 2$ and $n = 3$, respectively.

Define polynomial spaces on the faces of the elements to be:

$$R^k(\partial T) = \{\varphi \in L^2(\partial T) : \varphi|_F \in P^k(F) \quad \text{for all } F \subset \partial T\},$$

where ∂T denotes the boundary of T, and F denotes a face of T. The dimension of $R^k(\partial T)$ is $3(k+1)$ and $2(k+1)(k+2)$ for $n = 2$(triangles) and $n = 3$(tetrahedrons), respectively. We can now define the Raviart-Thomas-Nédélec elements. For each $k \geq 0$, let

$$RT^k(T) = \{\boldsymbol{\phi} + q\mathbf{x} : \mathbf{x} \in T \text{ where } \boldsymbol{\phi} \in (P^k(T))^n \text{ and } q \in P^k(T)\}.$$

It can be easily seen that the dimension of $RT^k(T)$ is given by

$$\dim RT^k(T) = \begin{cases} (k+1)(k+3) & \text{for } n = 2\ (triangles), \\ \frac{1}{2}(k+1)(k+2)(k+4) & \text{for } n = 3\ (tetrahedrons). \end{cases}$$

Theorem 4.8. *Let* $T \in \mathcal{T}_h$*. then*

$$\mathrm{div} P^k(T) + \mathrm{div} RT^k(T) = P^k(T).$$

Moreover, for any $\mathbf{v} \in RT^k(T)$

$$\mathbf{v} \cdot \mathbf{n}_T|_{\partial T} \in P^k(\partial T),$$

where $\mathbf{n}_T$ *denotes the outward unit normal from* T *on* ∂T*.*

Proof. Let $T \in \mathcal{T}_h$. The first statement is trivial from the definition of the polynomial and Raviart-Thomas-Nédélec spaces. Let $\mathbf{v} \in RT^k(T)$ and $\mathbf{x} \in \partial T$, then

$$(\mathbf{v} \cdot \mathbf{n}_T)(\mathbf{x}) = \boldsymbol{\phi}(\mathbf{x}) \cdot \mathbf{n}_T(\mathbf{x}) + q(\mathbf{x})\mathbf{x} \cdot \mathbf{n}_T(\mathbf{x}),$$

where $\boldsymbol{\phi} \in (P^k(T))^n$ and $q \in P^k(\partial T)$. Now $\mathbf{x} \cdot \mathbf{n}_T(\mathbf{x})$ is constant on each face $F \in \partial T$, and therefore $\mathbf{v} \cdot \mathbf{n}_T|_{\partial T} \in P^k(\partial T)$. ■

To uniquely define a function in $RT^k(T)$ we have:

Theorem 4.9. *Let $T \in \mathcal{T}_h$ and $\mathbf{v} \in RT^k(T)$. If*

$$\begin{aligned} \int_{\partial T} \mathbf{v} \cdot \mathbf{n}_T p \, ds &= 0 \quad \textit{for all } \varphi \in P^k(\partial T), \\ \int_T \mathbf{v} \cdot \boldsymbol{\varphi} \, d\mathbf{x} \, ds &= 0 \quad \textit{for all } \boldsymbol{\varphi} \in (P^{k-1}(T))^n, \end{aligned}$$

then $\mathbf{v} = 0$.

Proof. See (Brezzi and Fortin, 1991, proposition III.3.3). ■

Theorems 4.8 and 4.9 imply that we can use the following degrees of freedom to uniquely define a function $\mathbf{v} \in RT^k(T)$ (see Figure 4.1):

- The moments of order up to k of $\mathbf{v} \cdot \mathbf{n}_T$ on each face F of T, i.e.

$$\int_F \mathbf{v} \cdot \mathbf{n}_T \varphi \, ds \quad \varphi \in P^k(\partial T).$$

- The momentum of order up to $k-1$ of $\mathbf{v}$ on T, for $k > 0$, i.e.

$$\int_T \mathbf{v} \cdot \boldsymbol{\varphi} \, d\mathbf{x} \quad \boldsymbol{\varphi} \in (P^{k-1}(\partial T))^n.$$

4.2.5 The lowest order Raviart-Thomas element

The most interesting case from the computational point of view is the lowest order Raviart-Thomas element, i.e., $k = 0$, especially when we can not expect hight regularity of the solutions of the continuous problem. We start with defining a local basis function of RT^0 on a reference element.

Let $\hat{T}$ be the convex hull of L suitably chosen points $\hat{\mathbf{x}}_\ell, \ell = 1, \ldots, L$, that is

$$\hat{T} = \left\{ \hat{\mathbf{x}} = \sum_1^L \zeta_\ell \hat{\mathbf{x}}_\ell : 0 \le \zeta_\ell \le 1, \ \sum_1^L \zeta_\ell = 1 \right\}. \tag{4.2.21}$$

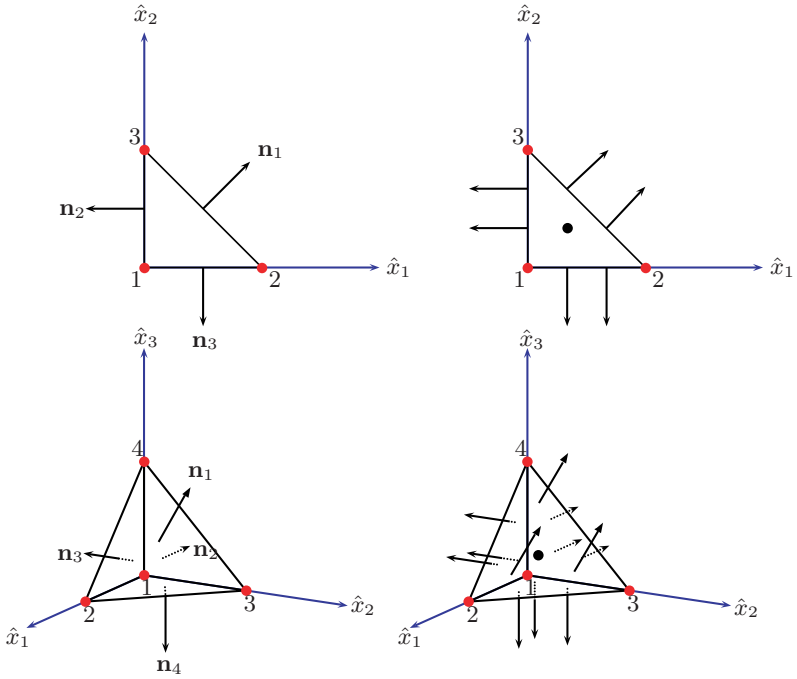


Figure 4.1. $RT^0(T)$ (left) and $RT^1(T)$ (right).

Define the affine map

$$\mathbf{x} = \mathbf{F}_n(\hat{\mathbf{x}}) = \mathbf{B}_n\hat{\mathbf{x}} + \mathbf{b}_n, \quad \hat{\mathbf{x}} \in \hat{T}, \tag{4.2.22}$$

where $\mathbf{B}_n \in \mathbb{R}^{n\times n}$ such that $\det \mathbf{B}_n > 0$, and $\mathbf{b}_n \in \mathbb{R}^n$.

Define $P^1(\hat{T})$ as the L-dimensional space of polynomials (for triangles $L = 3$ and for tetrahedrons $L = 4$) spanned by the basis functions $\hat{\varphi}_i$, $i = 1, \ldots, L$, such that

$$\hat{\varphi}_i(\hat{\mathbf{x}}_j) = \delta_{ij}. \tag{4.2.23}$$

Now, define $P^1(T)$ as the L-dimensional space spanned by

$$\varphi_i(\mathbf{x}) = \hat{\varphi}_i(\hat{\mathbf{x}}), \quad i = 1, \ldots, L. \tag{4.2.24}$$

It is well known that

$$\int_T \varphi_i \, d\mathbf{x} = \int_{\hat{T}} \hat{\varphi}_i \det \mathbf{B}_n \, d\hat{\mathbf{x}}. \tag{4.2.25}$$

Also

$$\nabla\varphi_i(\mathbf{x}) = \mathbf{B}_n^{-T}\nabla\hat{\varphi}(\hat{\mathbf{x}}) \quad \text{for all } \hat{\mathbf{x}} \in \hat{T}. \tag{4.2.26}$$

Since $\mathcal{V}$ consists of vectorial functions, the following subspaces are defined to approximate each component of functions in this space.

$$P^1_{-1}(\mathcal{T}_h) = \{\varphi \in L^2(\Omega) : \varphi|_T \in P^1(T) \text{ for all } T \in \mathcal{T}_h\}, \quad (4.2.27)$$

$$P^1_0(\mathcal{T}_h) = P^1_{-1}(\mathcal{T}_h) \cap H^1(\Omega), \quad (4.2.28)$$

$$P^1_D(\mathcal{T}_h) = \{\varphi \in P^1_0(\mathcal{T}_h) : \varphi = 0 \text{ on } \Gamma^D_{\mathbf{u}}\}. \quad (4.2.29)$$

Let $\hat{e}_i$, $i = 1, \ldots, I$, be the edges (n=2) or faces (n=3) of $\hat{T}$, and $RT^0(\hat{T})$ be the I-dimensional space of linear vectorial functions $\hat{\mathbf{u}}$ on $\hat{T}$ such that $\mathbf{n}_{\hat{T}} \cdot \hat{\mathbf{u}}$ is constant on $\hat{e}_i$, $i = 1, \ldots, I$. The basis functions for this space are $\hat{\mathbf{v}}_i$, $i = 1, \ldots, I$, such that

$$\int_{\hat{e}_j} \mathbf{n}_{\hat{T}} \cdot \hat{\mathbf{v}}_i \, d\hat{s} = \delta_{ij}, \qquad i, j = 1, \ldots, I. \quad (4.2.30)$$

Define $RT^0(T)$ be the space spanned by the basis functions

$$\mathbf{v}_i(\mathbf{x}) = (\det \mathbf{B}_n)^{-1} \mathbf{B}_n \hat{\mathbf{v}}_i(\hat{\mathbf{x}}), \qquad \hat{\mathbf{x}} \in \hat{T}, \quad (4.2.31)$$

that is,

$$RT^0(T) = \left\{ (\det \mathbf{B}_n)^{-1} \mathbf{B}_n \hat{\mathbf{u}}, \quad \hat{\mathbf{u}} \in RT^0(\hat{T}) \right\}. \quad (4.2.32)$$

Theorem 4.10. *Let* $\hat{\mathbf{u}} \in \mathbf{L}^2(\hat{T})$ *and* $\hat{\varphi} \in L^2(\hat{T})$.

$$\mathbf{u}(\mathbf{x}) = (\det \mathbf{B}_n)^{-1} \mathbf{B}_n \hat{\mathbf{u}}, \quad \varphi(\mathbf{x}) = \hat{\varphi}(\hat{\mathbf{x}}),$$

then the following equalities hold:

$$\int_T \mathbf{u} \cdot \nabla \varphi \, d\mathbf{x} = \int_{\hat{T}} \hat{\mathbf{u}} \cdot \nabla \hat{\varphi} \, d\hat{\mathbf{x}} \text{ for all } \hat{\mathbf{u}} \in \mathbf{L}^2(\hat{T}),\ \hat{\varphi} \in H^1(\hat{T}), \quad (4.2.33)$$

$$\int_T \varphi \nabla \cdot \mathbf{u} \, d\mathbf{x} = \int_{\hat{T}} \hat{\varphi} \nabla \cdot \hat{\mathbf{u}} \, d\hat{\mathbf{x}} \text{ for all } \hat{\varphi} \in L^2(\hat{T}),\ \hat{\mathbf{u}} \in H(\mathrm{div}; \hat{T}), \quad (4.2.34)$$

$$\int_{\partial T} \varphi \mathbf{n}_T \cdot \mathbf{u} \, ds = \int_{\partial \hat{T}} \hat{\varphi} \mathbf{n}_{\hat{T}} \cdot \hat{\mathbf{u}} \, d\hat{s} \text{ for all } \hat{\varphi} \in H^1(\hat{T}),\ \hat{\mathbf{u}} \in H(\mathrm{div}; \hat{T}), \quad (4.2.35)$$

where $\mathbf{n}_T$ *and* $\mathbf{n}_{\hat{T}}$ *are the outward normals to* ∂T *and* $\partial \hat{T}$*, respectively.*

Proof. For a proof, see (Thomas, 1977, proposition II-5.2 and II-5.4). ■

From equation (4.2.35) it follows that, if $\hat{\mathbf{u}} \in H(\mathrm{div}; \hat{T})$, then $\mathbf{u} \in H(\mathrm{div}; T)$ and

$$\nabla \cdot \mathbf{u}(\mathbf{x}) = (\det \mathbf{B}_n)^{-1} \nabla \cdot \hat{\mathbf{u}}(\hat{\mathbf{x}}). \quad (4.2.36)$$

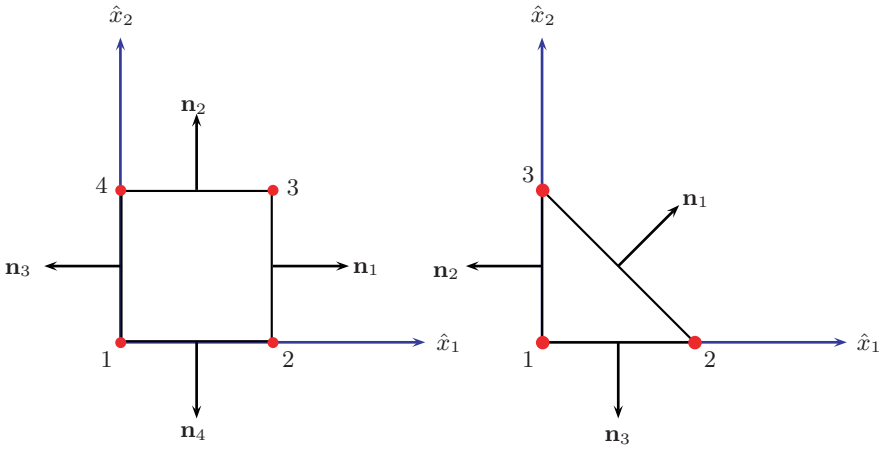


Figure 4.2. Two-dimensional mixed reference elements.

Note by Theorem 4.10 and relation (4.2.32), for every $\mathbf{u} \in RT^0(T)$, $\mathbf{n}_T \cdot \mathbf{u}$ is constant on the edges (n=2), or faces (n=3) e_i, $i = 1, \ldots, I$.
As an example of the two-dimensional space, we consider the triangle $\hat{T}_T$ with the coordinates

$$\hat{\mathbf{x}}_i : \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

The basis functions for $P^1(\hat{T}_T)$ and $RT^0(\hat{T}_T)$ can be obtained as:

$$\hat{\varphi}_i(\hat{\mathbf{x}}) : 1 - \hat{x}_1 - \hat{x}_2,\ \hat{x}_1,\ \hat{x}_2,$$

$$\hat{\mathbf{v}}_i(\hat{\mathbf{x}}) : \begin{pmatrix} \hat{x}_1 \\ \hat{x}_2 \end{pmatrix}, \begin{pmatrix} \hat{x}_1 - 1 \\ \hat{x}_2 \end{pmatrix}, \begin{pmatrix} \hat{x}_1 \\ \hat{x}_2 - 1 \end{pmatrix}.$$

Moreover, the affine map which transforms $\hat{T}_T$ to any triangle with vertices $\binom{x_i}{y_i}$, $i = 1, 2, 3$, is

$$F(\hat{\mathbf{x}}) = \begin{pmatrix} x_2 - x_1 & x_3 - x_1 \\ y_2 - y_1 & y_3 - y_1 \end{pmatrix} \begin{pmatrix} \hat{x}_1 \\ \hat{x}_2 \end{pmatrix} + \begin{pmatrix} x_1 \\ y_1 \end{pmatrix}.$$

As another example consider the rectangle $\hat{T}_R$ with

$$\hat{\mathbf{x}}_i : \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Define two functions

$$\begin{cases} \hat{N}_0(x) = 1 - x, \\ \hat{N}_1(x) = x. \end{cases} \tag{4.2.37}$$

Therefore, the basis function for $P^1(\hat{T})$ associated with the node $\hat{\mathbf{x}}_i$ is

$$\hat{\varphi}_i(\hat{\mathbf{x}}) = \hat{N}_{\hat{\mathbf{x}}_i(1)}(\hat{x}_1)\hat{N}_{\hat{\mathbf{x}}_i(2)}(\hat{x}_2).$$

The basis functions for $RT^0(\hat{T}_R)$ associated with $\mathbf{n}_i$, $i = 1, 2, 3, 4$, are

$$\hat{\mathbf{v}}_i(\hat{\mathbf{x}}) : \begin{pmatrix} \hat{x}_1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \hat{x}_2 \end{pmatrix}, \begin{pmatrix} \hat{x} - 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \hat{x}_2 - 1 \end{pmatrix},$$

respectively. Any parallelogram T with vertices $\binom{x_i}{y_i}$, $i = 1, 2, 3, 4$, can be defined with the transformation

$$F(\hat{\mathbf{x}}) = \begin{pmatrix} x_2 - x_1 & x_4 - x_1 \\ y_2 - y_1 & y_4 - y_1 \end{pmatrix} \begin{pmatrix} \hat{x}_1 \\ \hat{x}_2 \end{pmatrix} + \begin{pmatrix} x_1 \\ y_1 \end{pmatrix}.$$

In three-dimensional space, we consider two reference elements. Given a cube with the coordinates

$$\hat{\mathbf{x}}_i : \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix},$$

then the basis function associated with the node $\hat{\mathbf{x}}_i$ is taken as

$$\hat{\varphi}_i(\hat{\mathbf{x}}) = \hat{N}_{\hat{\mathbf{x}}_i(1)}(\hat{x}_1)\hat{N}_{\hat{\mathbf{x}}_i(2)}(\hat{x}_2)\hat{N}_{\hat{\mathbf{x}}_i(3)}(\hat{x}_3).$$

The Raviart-Thomas basis function associated with the normal vector $\mathbf{n}_i$, $i = 1, \ldots, 6$, is

$$\hat{\mathbf{v}}_i : \begin{pmatrix} \hat{x}_1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \hat{x}_2 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ \hat{x}_3 \end{pmatrix}, \begin{pmatrix} \hat{x}_1 - 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \hat{x}_2 - 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ \hat{x}_3 - 1 \end{pmatrix}.$$

The second example will be a tetrahedron $\hat{T}_T$ with the coordinates

$$\hat{\mathbf{x}}_i : \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix},$$

The basis functions for $P^1(\hat{T}_T)$ and $RT^0(\hat{T}_T)$ can be obtained as:

$$\hat{\varphi}_i(\hat{\mathbf{x}}) : 1 - \hat{x}_1 - \hat{x}_2 - \hat{x}_3,\ \hat{x}_1,\ \hat{x}_2,\ \hat{x}_3.$$

and

$$\hat{\mathbf{v}}_i :\ 2\begin{pmatrix} \hat{x}_1 \\ \hat{x}_2 \\ \hat{x}_3 \end{pmatrix}, 2\begin{pmatrix} \hat{x}_1 - 1 \\ \hat{x}_2 \\ \hat{x}_3 \end{pmatrix}, 2\begin{pmatrix} \hat{x}_1 \\ \hat{x}_2 - 1 \\ \hat{x}_3 \end{pmatrix}, 2\begin{pmatrix} \hat{x}_1 \\ \hat{x}_2 \\ \hat{x}_3 - 1 \end{pmatrix}.$$

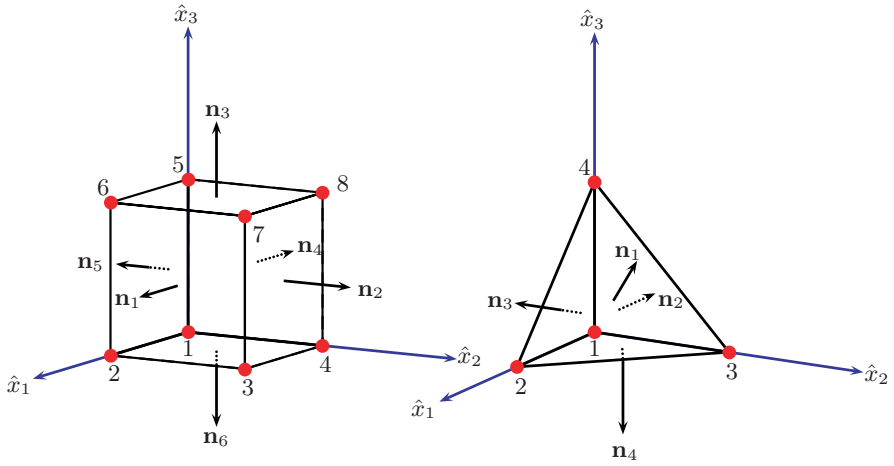


Figure 4.3. Three-dimensional mixed reference elements.

The detail and the overview of other possible choices for the reference element $\hat{T}$ can be found in (Kaasschieter and Huijben, 1992).

We define the Raviart-Thomas spaces

$$RT^0_{-1}(\mathcal{T}_h) = \{\mathbf{u} \in \mathbf{L}^2(\Omega) : \mathbf{u}|_T \in RT^0(T) \text{ for all } T \in \mathcal{T}_h\}, \quad (4.2.38)$$

$$RT^0_0(\mathcal{T}_h) = RT^0_{-1}(\mathcal{T}_h) \cap H(\mathrm{div};\Omega), \quad (4.2.39)$$

$$RT^0_{0,N}(\mathcal{T}_h) = RT^0_{-1}(\mathcal{T}_h) \cap H_N(\mathrm{div};\Omega). \quad (4.2.40)$$

Further, p in $L^2(\mathcal{T}_h)$ is approximated by piecewise constant functions. Therefore, let $M^0(T)$ be the one-dimensional space of constant scalar functions on T. Its basis function is ψ, where $\psi(\mathbf{x}) = 1$ for $\mathbf{x} \in T$.

Let $\mathbf{x}_i$, $i = 1, \ldots, I$, be numbered nodes of the triangulation $\{\mathbf{x} \in \mathcal{T}_h : \mathbf{x} \notin \overline{\Gamma}^D_{\mathbf{u}}\}$; $\mathcal{E}_h$ be the collection of edges $(n = 2)$ or faces $(n = 3)$ of sub-domains $T \in \mathcal{T}_h$; e_j, $j = 1, \ldots, J$, be the numbered edges $(n = 2)$ or faces $(n = 3)$ of $\{e \in \mathcal{T}_h : e \not\subset \overline{\Gamma}^D_p\}$ and T_k, $k = 1, \ldots K$, be the numbered sub-domains of $\mathcal{T}_h$. We assume that $\overline{\Gamma}^D_p$ is the union of some $e \in \mathcal{E}_h$. The same assumption holds for $\overline{\Gamma}^D_{\mathbf{u}}$.

The finite-dimensional space $RT^0_{0,N}(\mathcal{T}_h)$ is spanned by linearly independent vectorial basis functions $\mathbf{v}_i$, $i = 1, \ldots, J$, such that

$$\int_{e_j} \mathbf{n}_j \cdot \mathbf{v}_i \, ds = \delta_{ij}, \quad i, j = 1, \ldots, J,$$

where the normal vector $\mathbf{n}_j$ is the normal to e_j pointing from T_k to T_l, $k > l$, if $e_j = T_k \cap T_l$, and outward if $e_j \subset \overline{\Gamma}^D_p$.

The multiplier space $M^0_{-1}(\mathcal{T}_h)$ is defined as

$$M^0_{-1}(\mathcal{T}_h) = \{\lambda \in L^2(\Omega) : \lambda|_T \in M^0(T) \text{ for all } T \in \mathcal{T}_h\}. \tag{4.2.41}$$

Its basis functions are ψ_k, $k = 1, \ldots, K$, such that

$$\psi_k(\mathbf{x}) = \delta_{kl}, \quad \mathbf{x} \in T_l, \quad k, l = 1, \ldots, K. \tag{4.2.42}$$

4.2.6 The resulting saddle point problem

The variational problem (4.2.2) is approximated by

$$(\mathbf{u}_h, \mathbf{q}_h, p_h) \in (P^1_D(\mathcal{T}_h))^n \times RT^0_{0,N}(\mathcal{T}_h) \times M^0_{-1}(\mathcal{T}_h).$$

The functions $\mathbf{u}_h$, $\mathbf{q}_h$ and p_h are expressed as

$$\begin{aligned}
\mathbf{u}_h(\mathbf{x}, t) &= \sum_{i=1}^{I} \tilde{u_i}(t)\mathbf{w}_i(\mathbf{x}), \\
\mathbf{q}_h(\mathbf{x}, t) &= \sum_{j=1}^{J} \tilde{\mathbf{q}}_j(t)\mathbf{v}_j(\mathbf{x}) \\
p_h(\mathbf{x}, t) &= \sum_{k=1}^{K} \tilde{p}_k(t)\psi_k(\mathbf{x}).
\end{aligned}$$

Substitution in the discrete variational formulation, gives

$$\boxed{\mathfrak{A}\frac{d\mathbf{y}}{dt} + \mathfrak{B}\mathbf{y} = \mathfrak{F},} \tag{4.2.43}$$

where

$$\mathfrak{A} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \mathbf{B}^T & 0 & 0 \end{pmatrix}, \qquad \mathfrak{B} = \begin{pmatrix} \mathbf{A} & 0 & \mathbf{B} \\ 0 & \mathbf{C} & \mathbf{D} \\ 0 & \mathbf{D}^T & \mathbf{0} \end{pmatrix}$$

and

$$\begin{aligned}
\mathbf{y} &= [\tilde{\mathbf{u}}, \tilde{\mathbf{q}}, \tilde{\mathbf{p}}]^T, \\
\mathfrak{F} &= [\mathbf{F}, \mathbf{0}, \mathbf{0}]^T.
\end{aligned}$$

In the above formulation,

$$\begin{aligned}
\tilde{\mathbf{u}} &= [\tilde{u}_1 \cdots, \tilde{u}_I]^T, \\
\tilde{\mathbf{q}} &= [\tilde{q}_1, \cdots, \tilde{q}_J]^T, \\
\tilde{\mathbf{p}} &= [\tilde{p}_1, \cdots, \tilde{p}_K]^T, \\
\mathbf{A}_{ij} &= \int_\Omega \left(2\mu_s \boldsymbol{\mathcal{E}}(\mathbf{w}_i) : \boldsymbol{\mathcal{E}}(\mathbf{w}_j) + \lambda_s \nabla \cdot \mathbf{w}_i \nabla \cdot \mathbf{w}_j\right) \, d\mathbf{x}, \\
\mathbf{B}_{ij} &= -\int_\Omega \nabla \cdot \mathbf{w}_i \psi_j \, d\mathbf{x}, \\
\mathbf{C}_{ij} &= \frac{1}{K} \int_\Omega \mathbf{v}_i \cdot \mathbf{v}_j \, d\mathbf{x}, \\
\mathbf{D}_{ij} &= -\int_\Omega \nabla \cdot \mathbf{v}_j \psi_i \, d\mathbf{x}, \\
\mathbf{F}_i &= \int_{\Gamma_{\mathbf{u}}^N} \mathbf{g}_{\mathbf{u}}^N \cdot \mathbf{w}_i \, ds.
\end{aligned}$$

We shall use the implicit Euler scheme for time discretisation. Let Δt be the time step and $(\mathbf{u}_{h,n}, \mathbf{q}_{h,n}, p_{h,n})$ the approximation of the solution vector $(\mathbf{u}_h, \mathbf{q}_h, p_h)$ at $t = t_n = n\Delta t$. Then the system of equations resulting from backward Euler is

$$\begin{pmatrix} \mathbf{A} & 0 & \mathbf{B} \\ 0 & \Delta t\mathbf{C} & \Delta t\mathbf{D} \\ \mathbf{B}^T & \Delta t\mathbf{D}^T & \mathbf{0} \end{pmatrix} \begin{pmatrix} \tilde{\mathbf{u}}_n \\ \tilde{\mathbf{q}}_n \\ \tilde{\mathbf{p}}_n \end{pmatrix} = \begin{pmatrix} \mathbf{F} \\ \mathbf{0} \\ \mathbf{B}\tilde{\mathbf{u}}_{n-1} \end{pmatrix}. \tag{4.2.44}$$

Also it can be rewritten as

$$\begin{pmatrix} \mathbb{A} & \mathbb{B} \\ \mathbb{B}^T & \mathbf{0} \end{pmatrix} \begin{pmatrix} (\tilde{\mathbf{u}}_n, \tilde{\mathbf{q}}_n)^T \\ \tilde{\mathbf{p}}_n \end{pmatrix} = \begin{pmatrix} (\mathbf{F}, \mathbf{0})^T \\ \mathbf{B}\tilde{\mathbf{u}}_{n-1} \end{pmatrix}, \tag{4.2.45}$$

where

$$\mathbb{A} = \begin{pmatrix} \mathbf{A} & \mathbf{0} \\ \mathbf{0} & \Delta t\mathbf{C} \end{pmatrix}, \quad \mathbb{B} = \begin{pmatrix} \mathbf{B} \\ \Delta t\mathbf{D} \end{pmatrix}. \tag{4.2.46}$$

In (4.2.45), obviously $\mathbb{A}$ is symmetric positive definite because of he ellipticity of bilinear form $\mathbb{A}$. On the other hand, from the LBB condition it follows that the block $\mathbb{B}$ has full rank. Indeed, if $\tilde{\mathbf{p}} \in \mathbb{R}^K$ such that $\mathbb{B}\tilde{\mathbf{p}} = \mathbf{0}$, from LBB condition it follows that $\mathbb{B}(\mathbf{w}_i, \mathbf{v}_j; p_h) = 0$. Therefore

$$\mathbb{B}(\mathbf{u}_h, \mathbf{q}_h; p_h) = 0 \quad \text{for all } (\mathbf{u}_h, \mathbf{q}_h) \in \mathcal{V}_h \times \mathbf{W}_h,$$

and the LBB condition implies $p_h = 0$, i.e., $\tilde{p} = \mathbf{0}$.

From above we can see that the block matrix in (4.2.45) is symmetric and non-singular. However, this matrix is not positive definite. Indeed, take $\mathbf{p} \in \mathbb{R}^K$ and set $\mathbf{w} = \epsilon\mathbb{B}\mathbf{p} \in \mathbb{R}^{I+J}$. Then we have

$$(\mathbf{w}, \mathbf{p}) \begin{pmatrix} \mathbb{A} & \mathbb{B} \\ \mathbb{B}^T & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{w} \\ \mathbf{p} \end{pmatrix} = \mathbf{w}^T\mathbb{A}\mathbf{w} + 2\mathbf{w}^T\mathbb{B}\mathbf{p} = \epsilon\mathbf{p}^T \left(\epsilon\mathbb{B}^T\mathbb{A}\mathbb{B} + 2\mathbb{B}^T\mathbb{B}\right)\mathbf{p}. \tag{4.2.47}$$

The matrix $\mathbb{B}^T\mathbb{B}$ is symmetric positive definite and $\epsilon\mathbb{B}^T\mathbb{A}\mathbb{B}$ is positive definite if $\epsilon > 0$. If we choose $\epsilon < 0$ with $|\epsilon|$ sufficiently small, the right-hand side of (4.2.47) becomes negative. This shows that the system is an indefinite system. More precisely we have the following theorem.

Definition 4.11. *Let A be a linear transformation on $\mathbb{R}^n$ represented by a matrix $\mathbf{A}$. If there is a vector $0 \neq \mathbf{x} \in \mathbb{R}^n$ such that*

$$\mathbf{A}\mathbf{x} = \lambda\mathbf{x},$$

for some scalar λ, then λ is called the eigenvalue of $\mathbf{A}$ with corresponding (right) eigenvector $\mathbf{x}$. The eigenvalues of a matrix $\mathbf{A}$ are called its spectrum, and is denoted by $\mathrm{spec}(A)$.
For a square matrix $\mathbf{A}$, the square roots of the eigenvalues of $\mathbf{A}^T\mathbf{A}$ are called singular values of $\mathbf{A}$.

Theorem 4.12. *Let $0 < \lambda_{min} \leq \lambda_{max}$ be the minimum and maximum eigenvalues of $\mathbb{A}$ and let $0 \leq \sigma_{min} \leq \sigma_{max}$ be the minimum and maximum singular values of $\mathbb{B}$. then we have*

$$\mathrm{spec}(\begin{pmatrix} \mathbb{A} & \mathbb{B} \\ \mathbb{B}^T & \mathbf{0} \end{pmatrix}) \subset [\mu^-_{min}, \mu^-_{max}] \cup [\mu^+_{min}, \mu^+_{max}], \tag{4.2.48}$$

where

$$\begin{cases} \mu^-_{min} = 1/2\left(\lambda_{min} - \sqrt{\lambda^2_{min} + 4\sigma^2_{max}}\right) < 0 \\ \mu^-_{max} = 1/2\left(\lambda_{max} - \sqrt{\lambda^2_{max} + 4\sigma^2_{min}}\right) < 0 \\ \mu^+_{min} = \lambda_{min}, \\ \mu^+_{max} = 1/2\left(\lambda_{max} - \sqrt{\lambda^2_{max} + 4\sigma^2_{max}}\right) > 0. \end{cases}$$

Proof. See (Rusten and Winther, 1992, Lemma 2.1). ■

4.3 Hybridization of the mixed method

Fraeijs de Veubeke (Fraeijs de Veubeke, 1965) and (Fraeijs de Veubeke, 1977) introduced a hybrid method for the mixed formulation in order to simplify the solution of the algebraic system that must be solved in the procedure. In Kaasschieter and Huijben (1992) a mixed-hybrid finite element discretisation is used to solve an important class of problems in mathematical physics that involves equations of the form

$$\begin{cases} \mathbf{q} = -\mathbf{A}\nabla\mu, \\ \nabla \cdot \mathbf{q} = f, \end{cases}$$

where $\mathbf{A}$ is a symmetric and uniformly positive definite second order tensor. It can be seen that the mixed formulation of the above system leads to a saddle point problem. Using the hybridization technique, the mixed finite element method results in a

system of linear equations with a sparse and symmetric positive definite coefficients matrix.

Despite to this fact, the hybridization method reduces the number of degrees of freedom. Furthermore, in the computations we only have to compute inverses of element-wise block diagonal matrices.

In this section the hybridization technique is used for two-component model. First we introduce a hybridization procedure for the mixed formulation. This will simplify the solution of the algebraic system that must be solved in the procedure. The idea behind hybridization is to relax the continuity requirement for the variables $\mathbf{q}$. This will require to enlarge the Raviart-Thomas space in which $\mathbf{q}$ is sought and to introduce Lagrange multipliers to enforce the continuity of the normal component of $\mathbf{q}$ across the inter-element boundaries.

Define

$$\mathcal{E}_h^{\partial} = \{e \in \mathcal{E}_h : e \subset \Gamma\}. \tag{4.3.1}$$

We assume that Γ_p^D is the union of some $e \in \mathcal{E}_h^{\partial}$.

The hybrid formulation will make use of Lagrangian multipliers belonging to the space $L^2(\mathcal{E}_h)$ that is defined to be the product space

$$L^2(\mathcal{E}_h) = \prod_{T \in \mathcal{T}_h} L^2(\partial T). \tag{4.3.2}$$

Recall that $M^0(e)$, $e \in \mathcal{E}_h$, is the space of constant functions on e. Define the multiplier spaces

$$M_{-1}^0(\mathcal{E}_h) = \{\lambda = (\lambda_e)_{e \in \mathcal{E}_h} \in H^{1/2}(\bigcup_{e \in \mathcal{E}_h} e) : \lambda_e \in M^0(e) \text{ for all } e \in \mathcal{E}_h\}, \tag{4.3.3}$$

$$M_{-1,D}^0(\mathcal{E}_h) = \{\lambda \in M_{-1}^0(\mathcal{E}_h) : \lambda = 0 \quad \text{on} \quad \Gamma_p^D\}. \tag{4.3.4}$$

The following lemma is an immediate consequence of the above definitions.

Lemma 4.13. *Suppose* $\mathbf{q} \in RT_{-1}^0(\mathcal{T}_h)$, *then* $\mathbf{q} \in RT_{0,N}^0(\mathcal{T}_h)$ *if, and only if,*

$$\sum_{T \in \mathcal{T}_h} \int_{\partial T} \lambda \mathbf{n}_T \cdot \mathbf{q} \, ds = 0 \quad \textit{for all } \lambda \in M_{-1,D}^0(\mathcal{E}_h).$$

A spatial semi-discrete approximation by considering the hybridization technique is:

Find $(\mathbf{u}_h, \mathbf{q}_h, p_h, \lambda_h)(\cdot, t) \in (P_D^1(\mathcal{T}_h))^n \times RT_{-1}^0(\mathcal{T}_h) \times M_{-1}^0(\mathcal{T}_h) \times M_{-1,D}^0(\mathcal{E}_h)$

such that:

$$\begin{cases} \displaystyle\int_\Omega (2\mu_s \boldsymbol{\mathcal{E}}(\mathbf{u}_h) : \boldsymbol{\mathcal{E}}(\bar{\mathbf{u}}_h) + \lambda_s \nabla\cdot\mathbf{u}_h \nabla\cdot\bar{\mathbf{u}}_h)\, d\mathbf{x} - \int_\Omega p_h \nabla\cdot\bar{\mathbf{u}}_h\, d\mathbf{x} \\ \quad = \displaystyle\int_{\Gamma_{\mathbf{u}}^N} \mathbf{g}_{\mathbf{u}}^N \cdot \bar{\mathbf{u}}_h\, ds, & (4.3.5a) \\ \displaystyle\frac{1}{K}\int_\Omega \mathbf{q}_h\cdot\bar{\mathbf{q}}_h\, d\mathbf{x} - \sum_{T\in\mathcal{T}_h}\left(\int_T p_h \nabla\cdot\bar{\mathbf{q}}_h\, d\mathbf{x} - \int_{\partial T}\lambda_h \mathbf{n}_T\cdot\bar{\mathbf{q}}_h\, ds\right) = 0, & (4.3.5b) \\ -\displaystyle\sum_{T\in\mathcal{T}_h}\int_T \nabla\cdot\mathbf{q}_h\bar{p}_h\, d\mathbf{x} - \int_\Omega \frac{\partial \nabla\cdot\mathbf{u}_h}{\partial t}\bar{p}_h\, d\mathbf{x} = 0, & (4.3.5c) \\ \displaystyle\sum_{T\in\mathcal{T}_h}\int_{\partial T}\mathbf{n}_T\cdot\mathbf{q}_h\bar{\lambda}_h\, ds = 0, & (4.3.5d) \end{cases}$$

for all test functions $\left(\bar{\mathbf{u}}_h, \bar{\mathbf{q}}_h, \bar{p}_h, \bar{\lambda}_h\right) \in (P_D^1(\mathcal{T}_h))^n \times RT_{-1}^0(\mathcal{T}_h) \times M_{-1}^0(\mathcal{T}_h) \times M_{-1,D}^0(\mathcal{E}_h)$ and $t > 0$.

Let $\mathbf{x}_i$, $i = 1,\ldots,I$, be numbered nodes of the triangulation $\{\mathbf{x}\in\mathcal{T}_h : \mathbf{x}\notin\overline{\Gamma}_{\mathbf{u}}^D\}$; T_k, $k = 1,\ldots,K$, be numbered sub-domains of $\mathcal{T}_h$ and $e_j^{(T)}$, $j = 1,\ldots,J^{(T)}$, be the edges $(n = 2)$ or faces $(n = 3)$ of T for each $T\in\mathcal{T}_h$.

Recall that the finite-dimensional space $RT_{-1}^0(\mathcal{T}_h)$ is spanned by linearly independent vectorial basis functions $\mathbf{v}_j^{(T)}$, $j = 1,\ldots,J^{(T)}$, $T\in\mathcal{T}_h$, such that $\mathbf{v}_j^{(T)}$ has its support in T and

$$\int_{e_{j'}^{(T)}} \mathbf{n}_t\cdot\mathbf{v}_j^{(T)}\, ds = \delta_{jj'}, \quad j,j' = 1,\ldots,J^{(T)}.$$

Thus a function $\mathbf{q}\in RT_{-1}^0(\mathcal{T}_h)$ has $J^{(T)}$ degrees of freedom per sub-domain $T\in\mathcal{T}_h$ and in total $J = \sum_{T\in\mathcal{T}_h} J^{(T)}$ degrees of freedom in $\mathcal{T}_h$. The degrees of freedom of $\mathbf{q}$ in the sub-domain $T\in\mathcal{T}_h$ are equal to

$$\int_{e_j^{(T)}} \mathbf{n}_T\cdot\mathbf{q}\, ds, \quad j = 1,\ldots J^{(T)}.$$

Recall that the finite-dimensional space $M_{-1}^0(\mathcal{T}_h)$ is spanned by the linearly independent scalar basis functions ψ_k, $k = 1,\ldots,K$, such that (4.2.42) holds.

Let e_l, $l = 1,\ldots,L$, be the numbered edges $(n = 2)$ or faces $(n = 3)$ of $\{e\in\mathcal{E}_h : e\not\subset\overline{\Gamma}_p^D\}$. The finite-dimensional space $M_{-1,D}^0(\mathcal{E}_h)$ is spanned by the linearly independent scalar basis functions η_l, $l = 1,\ldots,L$, such that

$$\eta_l(\mathbf{x}) = \delta_{ll'}, \quad \mathbf{x}\in e_{l'}, \quad l,l' = 1,\ldots,L.$$

Therefore a function $\lambda \in M^0_{-1,D}(\mathcal{E}_h)$ has one degree of freedom per edge e_l, $l = 1, \ldots, L$, which is equal to its constant value on e_k.

Now by definition, functions $\mathbf{u}_h$, $\mathbf{q}_h$, p and λ_h are expressed as

$$\begin{aligned}
\mathbf{u}_h(\mathbf{x},t) &= \sum_{i=1}^{I} \tilde{u}_i(t)\mathbf{w}_i(\mathbf{x}),\\
\mathbf{q}_h(\mathbf{x},t) &= \sum_{j=1}^{J} \tilde{\mathbf{q}}_j(t)\mathbf{v}_j(\mathbf{x}),\\
p_h(\mathbf{x},t) &= \sum_{k=1}^{K} \tilde{p}_k(t)\psi_k(\mathbf{x}),\\
\lambda_h(\mathbf{x},t) &= \sum_{\ell=1}^{L} \tilde{\lambda}_\ell(t)\eta_l(\mathbf{x}).
\end{aligned}$$

Substituting this in the mixed-hybrid variational formulation gives

$$\boxed{\mathfrak{A}\frac{d\mathbf{y}}{dt} + \mathfrak{B}\mathbf{y} = \mathfrak{F},} \tag{4.3.6}$$

where $\mathfrak{A}$ and $\mathfrak{B}$ are

$$\mathfrak{A} = \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{B}^T & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \end{pmatrix}, \quad \mathfrak{B} = \begin{pmatrix} \mathbf{A} & \mathbf{0} & \mathbf{B} & \mathbf{0} \\ \mathbf{0} & \mathbf{C} & \mathbf{D} & \mathbf{E} \\ \mathbf{0} & \mathbf{D}^T & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{E}^T & \mathbf{0} & \mathbf{0} \end{pmatrix} \quad \text{and} \quad \begin{cases} \mathfrak{F} = & [\mathbf{F}, \mathbf{0}, \mathbf{0}, \mathbf{0}]^T, \\ \mathbf{y} = & \left[\tilde{\mathbf{u}}, \tilde{\mathbf{q}}, \tilde{\boldsymbol{\mu}}, \tilde{\boldsymbol{\lambda}}\right]^T. \end{cases}$$

In the above formulations,

$$\begin{aligned}
\tilde{\mathbf{u}} &= [\tilde{u}_1 \cdots, \tilde{u}_{nI}]^T,\\
\tilde{\mathbf{q}} &= [\tilde{q}_1, \cdots, \tilde{q}_J]^T,\\
\tilde{\mathbf{p}} &= [\tilde{p}_1, \cdots, \tilde{p}_K]^T,\\
\tilde{\boldsymbol{\lambda}} &= [\tilde{\lambda}_1, \cdots, \tilde{\lambda}_L]^T,\\
\mathbf{A}_{ij} &= \int_\Omega (2\mu_s \boldsymbol{\mathcal{E}}(\mathbf{w}_i) : \boldsymbol{\mathcal{E}}(\mathbf{w}_j) + \lambda_s \nabla\cdot\mathbf{w}_i \nabla\cdot\mathbf{w}_j)\, d\mathbf{x},\\
\mathbf{B}_{ij} &= -\int_{T_j} \nabla\cdot\mathbf{w}_i\, d\mathbf{x},\\
\mathbf{C}_{ij} &= \frac{1}{K}\int_\Omega \mathbf{v}_i\cdot\mathbf{v}_j\, d\mathbf{x},\\
\mathbf{D}_{ij} &= -\int_{T_j} \nabla\cdot\mathbf{v}_i\, d\mathbf{x},
\end{aligned}$$

$$\begin{aligned}\mathbf{E}_{ik} &= \int_{e_k} \mathbf{n}_i \cdot \mathbf{v}_i \, ds, \\ \mathbf{F}_i &= \int_{\Gamma_{\mathbf{u}}^N} \mathbf{g}_{\mathbf{u}}^N \cdot \mathbf{w}_i \, ds.\end{aligned}$$

Theorem 4.14. $(\mathbf{D}|\mathbf{E})^T\mathbf{C}^{-1}(\mathbf{D}|\mathbf{E})$ *is a symmetric positive definite matrix.*

Proof. $\mathbf{C}$ is symmetric positive definite and $(\mathbf{D}|\mathbf{E})^T\mathbf{C}^{-1}(\mathbf{D}|\mathbf{E})$ is symmetric positive semi-definite. To prove the positive-definiteness, we need to show that $(\mathbf{D}|\mathbf{E})$ has full rank. Suppose

$$(\mathbf{D}|\mathbf{E})\left(\tilde{\mathbf{p}}, \tilde{\boldsymbol{\lambda}}\right)^T = 0 \Rightarrow \mathbf{D}\tilde{\mathbf{p}} + \mathbf{E}\tilde{\boldsymbol{\lambda}} = 0.$$

But

$$\begin{aligned}
& \mathbf{D}\tilde{\mathbf{p}} + \mathbf{E}\tilde{\boldsymbol{\lambda}} = 0 \Leftrightarrow \mathbf{v}^T(\mathbf{D}\tilde{\mathbf{p}} + \mathbf{E}\tilde{\boldsymbol{\lambda}}) = 0 \quad \text{for all } \mathbf{v} \in \mathbb{R}^J \\
\Leftrightarrow \quad & \sum_{T\in\mathcal{T}_h} \left(\int_T p_h \nabla \cdot \mathbf{v}_h \, d\mathbf{x} - \int_{\partial T} \lambda_h \mathbf{n}_T \cdot \mathbf{v}_h \, ds \right) = 0 \quad \text{for all } \mathbf{v}_h \in RT^0_{-1}(\mathcal{T}_h) \\
\Leftrightarrow \quad & \sum_{T\in\mathcal{T}_h} \int_{\partial T} (p_h - \lambda_h)\mathbf{n}_T \cdot \mathbf{v}_h \, ds = 0 \quad \text{for all } \mathbf{v}_h \in RT^0_{-1}(\mathcal{T}_h) \\
\Leftrightarrow \quad & p_h = \lambda_h \text{ on } \partial T \quad \text{for all } T \in \mathcal{T}_h \Leftrightarrow p_h = 0 \text{ in } \Omega, \quad \lambda_h = 0 \text{ on } \bigcup_{e\in\mathcal{E}_h} e \\
\Leftrightarrow \quad & \tilde{\mathbf{p}} = \mathbf{0}, \quad \tilde{\boldsymbol{\lambda}} = \mathbf{0},
\end{aligned}$$

Therefore we have

$$\left(\mathbf{D}\tilde{\mathbf{p}} + \mathbf{E}\tilde{\boldsymbol{\lambda}}\right)^T \mathbf{C}^{-1} \left(\mathbf{D}\tilde{\mathbf{p}} + \mathbf{E}\tilde{\boldsymbol{\lambda}}\right) > 0 \tag{4.3.7}$$

for all $(\tilde{\mathbf{p}}, \tilde{\boldsymbol{\lambda}}) \in \mathbb{R}^{K+L}\backslash\{\mathbf{0}\}$. ■

In the sequel the hybridization technique will be proceeded. Note that the system (4.3.6) can be considered as

$$\begin{cases} \mathbf{A}\tilde{\mathbf{u}} + \mathbf{B}\tilde{\mathbf{p}}^l = \mathbf{F}, \\ \mathbf{C}\tilde{\mathbf{q}} + (\mathbf{D}|\mathbf{E}) \begin{pmatrix} \tilde{\mathbf{p}} \\ \tilde{\boldsymbol{\lambda}} \end{pmatrix} = \mathbf{0}, \\ \begin{pmatrix} \mathbf{B}^T \\ \mathbf{0} \end{pmatrix} \dfrac{d}{dt}\tilde{\mathbf{u}} + (\mathbf{D}|\mathbf{E})^T\tilde{\mathbf{q}} = \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \end{pmatrix} \end{cases} \tag{4.3.8}$$

In the system (4.3.8) $\mathbf{C}$ is a symmetric positive definite matrix and can be inverted at the finite element level. Therefore the second equation in (4.3.8) implies

$$\boxed{\tilde{\mathbf{q}} = -\mathbf{C}^{-1}(\mathbf{D}|\mathbf{E}) \begin{pmatrix} \tilde{\mathbf{p}} \\ \tilde{\boldsymbol{\lambda}} \end{pmatrix}.} \tag{4.3.9}$$

Using (4.3.9) and the third equation in (4.3.8) we get

$$\begin{pmatrix} \mathbf{B}^T \\ \mathbf{0} \end{pmatrix} \frac{d}{dt}\tilde{\mathbf{u}} - (\mathbf{D}|\mathbf{E})^T\mathbf{C}^{-1}(\mathbf{D}|\mathbf{E}) \begin{pmatrix} \tilde{\mathbf{p}} \\ \tilde{\boldsymbol{\lambda}} \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \end{pmatrix}. \tag{4.3.10}$$

In the next step we solve the above equation for $\tilde{\mathbf{p}}$. To do this, we need to state the following lemma.

Lemma 4.15. $\mathbf{D}^T\mathbf{C}^{-1}\mathbf{D}$ *is a symmetric positive definite matrix.*

Proof. Since $\mathbf{C}$ is a symmetric positive definite matrix, $\mathbf{D}^T\mathbf{C}^{-1}\mathbf{D}$ is symmetric positive semi-definite. In order to prove that this matrix is positive definite, we need to find the null space of it.
Let $\mathbf{D}\tilde{\mathbf{p}} = 0$, then

$$\sum_{T\in\mathcal{T}_h} \int_T p_h \nabla\cdot\mathbf{v}_h \, d\mathbf{x} = 0 \;\text{ for all }\; \mathbf{v}_h \in RT^0_{-1}(\mathcal{T}_h).$$

$\mathbf{v}_h$ is assumed to be continuous inside each element T, therefore the above summation will reduce to each element T. With an appropriate choice of $\mathbf{v}_h$, we can take $\nabla\cdot\mathbf{v}_h$ to be equal to 1 in T, therefore we have

$$\int_T p_h \, d\mathbf{x} = 0 \quad \text{for all } \; T \in \mathcal{T}_h.$$

Hence

$$p_h|_T = 0 \quad \text{for all } \; T \in \mathcal{T}_h.$$

This results in the symmetric positive definiteness of $\mathbf{D}^T\mathbf{C}^{-1}\mathbf{D}$. ■

Now by applying the above lemma, $\tilde{\mathbf{p}}$ can be derived as

$$\boxed{\tilde{\mathbf{p}} = (\mathbf{D}^T\mathbf{C}^{-1}\mathbf{D})^{-1}\left(-\mathbf{D}^T\mathbf{C}^{-1}\mathbf{E}\tilde{\boldsymbol{\lambda}} + \mathbf{B}^T\frac{d}{dt}\tilde{\mathbf{u}}\right).} \tag{4.3.11}$$

If we substitute (4.3.11) in system (4.3.10), then this system reduces to

$$\boxed{\begin{pmatrix} \mathbf{A}\tilde{\mathbf{u}} \\ \mathbf{0} \end{pmatrix} + \begin{pmatrix} \mathfrak{A}_1 & \mathfrak{A}_2 \\ \mathfrak{A}_2^T & -\mathfrak{A}_3 \end{pmatrix} \begin{pmatrix} \frac{d}{dt}\tilde{\mathbf{u}} \\ \tilde{\boldsymbol{\lambda}} \end{pmatrix} = \begin{pmatrix} \mathbf{F} \\ \mathbf{0} \end{pmatrix},} \tag{4.3.12}$$

where $\mathfrak{A}_1, \mathfrak{A}_1$ and $\mathfrak{A}_3$ are

$$\mathfrak{A}_1 = \mathbf{B}(\mathbf{D}^T\mathbf{C}^{-1}\mathbf{D})^{-1}\mathbf{B}^T, \tag{4.3.13}$$

$$\mathfrak{A}_2 = -\mathbf{B}(\mathbf{D}^T\mathbf{C}^{-1}\mathbf{D})^{-1}\mathbf{D}^T\mathbf{C}^{-1}\mathbf{E}, \tag{4.3.14}$$

$$\mathfrak{A}_3 = -\mathbf{E}^T\mathbf{C}^{-1}\mathbf{D}(\mathbf{D}^T\mathbf{C}^{-1}\mathbf{D})^{-1}\mathbf{D}^T\mathbf{C}^{-1}\mathbf{E} + \mathbf{E}^T\mathbf{C}^{-1}\mathbf{E}. \tag{4.3.15}$$

Remark 4.16. *Note that in computation of $\mathfrak{A}_1$, $\mathfrak{A}_2$ and $\mathfrak{A}_3$, the inverse of the matrix $\mathbf{D}\mathbf{C}^{-1}\mathbf{D}$ is needed.*

Remark 4.17. *From Theorem 4.14 it follows that*

$$\boldsymbol{\eta}^T\mathfrak{A}_3\boldsymbol{\eta} = (\mathbf{D}\boldsymbol{\eta}_1 + \mathbf{E}\boldsymbol{\eta}_2)^T\,\mathbf{C}^{-1}\,(\mathbf{D}\boldsymbol{\eta}_1 + \mathbf{E}\boldsymbol{\eta}_2) > 0 \;\; \textit{for all} \;\; \boldsymbol{\eta}_2 \in \mathbb{R}^K\backslash\{0\}, \tag{4.3.16}$$

where

$$\boldsymbol{\eta}_1 = -(\mathbf{D}\mathbf{C}^{-1}\mathbf{D})^{-1}\mathbf{D}^T\mathbf{C}^{-1}\mathbf{E}\boldsymbol{\eta}_2, \quad \boldsymbol{\eta} = (\boldsymbol{\eta}_1, \boldsymbol{\eta}_2).$$

Therefore $\mathfrak{A}_3$ is a symmetric positive definite matrix.

Remark 4.18. *By using the above remark, we can take one more step to solve the system for*

$$\tilde{\boldsymbol{\lambda}} = \mathfrak{A}_3^{-1}\mathfrak{A}_2^T\tilde{\mathbf{u}}, \tag{4.3.17}$$

hence the system (4.3.12) *is reduced to*

$$\boxed{\left(\mathfrak{A}_1 + \mathfrak{A}_2\mathfrak{A}_3^{-1}\mathfrak{A}_2^T\right)\frac{d}{dt}\tilde{\mathbf{u}} + \mathbf{A}\tilde{\mathbf{u}} = \mathbf{F}.} \tag{4.3.18}$$

Letting Δt be the time step and $(\tilde{\mathbf{u}}_n, \tilde{\boldsymbol{\lambda}}_n)$ the approximation of the solution vector $(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\lambda}})$ at $t = t_n = n\Delta t$. Then the nonlinear system of equations (4.3.12) resulting from backward Euler is:

$$\begin{pmatrix} \mathbf{A} + \mathfrak{A}_1/\Delta t & \mathfrak{A}_2 \\ \mathfrak{A}_2^T & -\Delta t\mathfrak{A}_3 \end{pmatrix}\begin{pmatrix} \tilde{\mathbf{u}}_{n+1} \\ \tilde{\boldsymbol{\lambda}}_{n+1} \end{pmatrix} = \begin{pmatrix} \mathbf{F} + \mathfrak{A}_1\tilde{\mathbf{u}}_n/\Delta t \\ \mathfrak{A}_2^T\tilde{\mathbf{u}}_n \end{pmatrix}. \tag{4.3.19}$$

Remark 4.19. *Frijns (Frijns, 2001, page 54) has shown that oscillations in the solution of discretised system*

$$\left(\mathfrak{A}_1 + \mathfrak{A}_2\mathfrak{A}_3^{-1}\mathfrak{A}_2^T + \Delta t\mathbf{A}\right)\tilde{\mathbf{u}}_{n+1} = \Delta t\mathbf{F} + \left(\mathfrak{A}_1 + \mathfrak{A}_2\mathfrak{A}_3^{-1}\mathfrak{A}_2^T\right)\tilde{\mathbf{u}}_{n+1}$$

can occur when matrix $\mathfrak{A}_1 + \mathfrak{A}_2\mathfrak{A}_3^{-1}\mathfrak{A}_2^T + \Delta t\mathbf{A}$ is not an M-matrix. This matrix will be an M-matrix if

$$\Delta t > \Delta t_{crit} = \frac{h^2}{6K(2\mu_s + \lambda_s)}, \tag{4.3.20}$$

where h is the mesh size.

4.4 Numerical Simulations

In this section the element contributions to the matrices and right-hand sides in (4.3.12) are computed. Remember the given triangulation $\mathcal{T}_h$ of Ω and the reference element $\hat{T}$ in (4.2.21).

The element contribution to the elasticity matrix $\mathbf{A}$ and $\mathbf{B}$ can be calculated in a standard way. To calculate the element contribution to the matrices $\mathbf{C}$ we need to consider the following analysis. Considering (4.2.31) we have

$$\left(\mathbf{C}^{(T)}_{J^{(T)}\times J^{(T)}}\right)_{ij} = \int_T \mathbf{v}_i^{(T)} \cdot \mathbf{v}_j^{(T)} d\mathbf{x} = \int_{\hat{T}} \hat{\mathbf{C}}^{(T)} \hat{\mathbf{v}}_i \cdot \hat{\mathbf{v}}_j d\,\hat{\mathbf{x}}, \tag{4.4.1}$$

where

$$\hat{\mathbf{C}}^{(T)}(\hat{x}) = (\det \mathbf{B}_n)^{-1} \mathbf{B}_n^T \mathbf{B}_n$$

and

$$\hat{\mathbf{v}}_i(\hat{\mathbf{x}}) = (\det \mathbf{B}_n)\mathbf{B}_n^{-1}\mathbf{v}_i^{(T)}(\mathbf{x}), \quad \mathbf{x} \in T.$$

Note that the local basis functions $\hat{\mathbf{v}}_i, i = 1, ..., J^{(T)}$, only depend on the reference element $\hat{T}$. If the notations

$$\hat{\mathbf{v}}_i(\hat{\mathbf{x}}) = [\hat{v}_{ik}(\hat{\mathbf{x}})]_{k=1,...,n} \quad \text{and} \quad \hat{\mathbf{C}}^{(T)} = \left[\hat{c}_{kl}^{(T)}\right]_{k,l=1,...,n}$$

are used, then

$$\int_{\hat{T}} \hat{\mathbf{C}}^{(T)} \hat{\mathbf{v}}_i \cdot \hat{\mathbf{v}}_j d\hat{\mathbf{x}} = \sum_{k=1}^{n}\sum_{l=1}^{n} \hat{c}_{kl}^{(T)} \left(\mathbf{A}_{kl}\right)_{ij}, \tag{4.4.2}$$

where the matrices

$$\left((\mathbf{A}_{kl})_{J^{(T)}\times J^{(T)}}\right)_{ij} = \int_{\hat{T}} \hat{v}_{ik}\hat{v}_{jl}\, d\hat{\mathbf{x}} \tag{4.4.3}$$

only depend on the reference element $\hat{T}$. Note that $\hat{c}_{kl}^{(T)} = \hat{c}_{lk}^{(T)}$ and $\mathbf{A}_{kl} = \mathbf{A}_{lk}$, thus

$$\boxed{\left(\mathbf{C}^{(T)}_{J^{(T)}\times J^{(T)}}\right)_{ij} = \sum_{k=1}^{n} \hat{c}_{kk}^{(T)} \left(\mathbf{A}_{kk}\right)_{ij} + \sum_{k=1}^{n}\sum_{l=1}^{n-1} \hat{c}_{kl}^{(T)} \left(\mathbf{A}_{kl} + \mathbf{A}_{lk}\right)_{ij},} \tag{4.4.4}$$

where all matrices in the summations are symmetric. In (Kaasschieter and Huijben, 1992) an overview of the matrices $\mathbf{A}_{kk}$ and $\mathbf{A}_{kl} + \mathbf{A}_{lk}$, $k \neq l$, corresponding to various choice of the reference element $\hat{T}$ is given.

Using Green's formula, (4.2.30) and (4.2.35), simple formulas can be derived for the element contributions of the remaining matrices and right-hand sides in (4.3.12), namely

$$\boxed{\begin{aligned} \left(\mathbf{D}^{(T)}_{J^{(T)}\times 1}\right)_i &= -\int_T \nabla \cdot \mathbf{v}_i^{(T)}\, d\mathbf{x} = -1, \\ \left(\mathbf{E}^{(T)}_{J^{(T)}\times J^{(T)}}\right)_{ik} &= \int_{e_k^{(T)}} \mathbf{n}_T \cdot \mathbf{v}_i^{(T)}\, ds = \delta_{ik}, \end{aligned}} \tag{4.4.5}$$

The computation of $(\mathbf{D}^T\mathbf{C}^{-1}\mathbf{D})^{-1}$ is essential when determining the matrices $\mathfrak{A}_i$, $(i = 1, 2, 3)$ in (4.3.13)-(4.3.15). This matrix is a diagonal matrix and it can thus be computed at the finite element level. The matrices $\mathfrak{A}_i$ are obtained by assembling their element contributions.

4.4.1 Example 1: One-dimensional confined compression problem

In this section the numerical solutions are calculated for given examples. To verify the method, solutions are compared with the analytical solutions from chapter 3.

A one-dimensional confined compression experiment is considered. The homogeneous sample with the diameter of 4 mm and the height of approximately $L = 1$ mm is put in an insulating conforming ring. A piston on the top of the sample is loaded mechanically. Figure 4.4 illustrate the experimental setup. In this experiment, we apply load on the piston to be equal to $f(t) = -f_0\mathcal{H}(t - t_0)$, with $\mathcal{H}(t - t_0)$ the Heaviside function and $f_0 > 0$. The following parameters are taken:

Parameter	Unit	Value
$2\mu_s + \lambda_s$	MPa	4×10^3
K	$\mathrm{m}^4\ \mathrm{N}^{-1}\ \mathrm{s}^{-1}$	1.0×10^{-18}
φ		0.7
f_0	MPa	5

Table 4.1. Material parameters

We use a rectangle in which only vertical displacement (direction of force) is allowed with 40 vertical elements and one horizontal element. The variation of water pressure, displacement along the y axis and the fluid flow are shown in Figure 4.4. For $t \to t_o^+$, the pressure shows a large gradients. This is due to the fact that the Dirichlet boundary condition $p = 0$ at $y = L$ contradicts with the asymptotic behaviour $p \to f_0$ as $t \to t_0^+$. Frijns (Frijns, 2001, page 54) has shown that the time step influences the choice of an initial grid. In fact, the time step should be larger than the critical time step using above material parameters

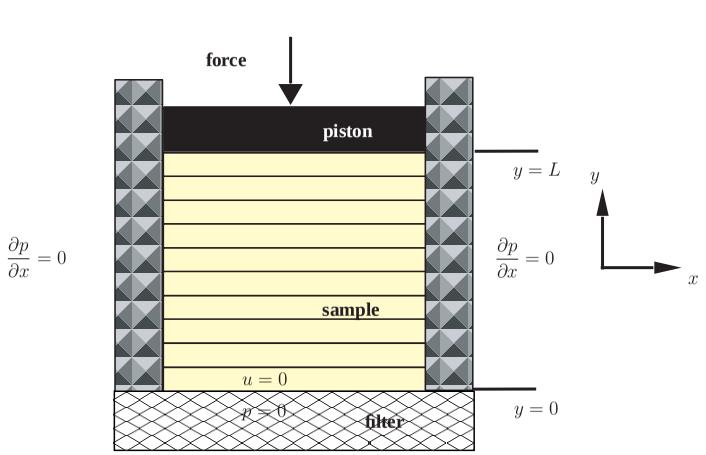
$$\Delta t \geq \Delta_{crit} t = \frac{h_y^2}{6K(2\mu_s + \lambda_s)}.$$

This shows that to have a smaller time step we do need to refine our mesh. The L^2-norm for the global error in the displacement solution at the final time are also calculated and it appears that the error is $\mathcal{O}(\Delta t)$ and $\mathcal{O}(h^2)$ (Frijns, 2001).

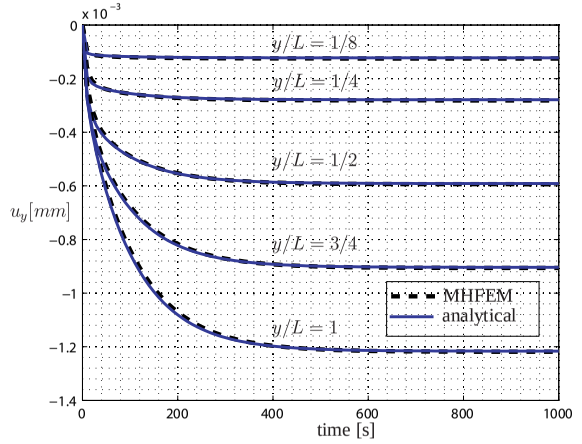
4.4.2 Example 2: Two-dimensional footing problem

The second example is a two-dimensional footing problem as given in (Murad and Loula, 1994). The simulation domain is a 8×5 mm block of porous medium. At the basis of this domain the medium is assumed to be fixed and impervious, while at the upper left part of the domain (fourth of the total length) we apply load on the $f(t) = -f_0\mathcal{H}(t - t_0)$, with $\mathcal{H}(t - t_0)$ the Heaviside function and $f_0 = 5$ MPa.

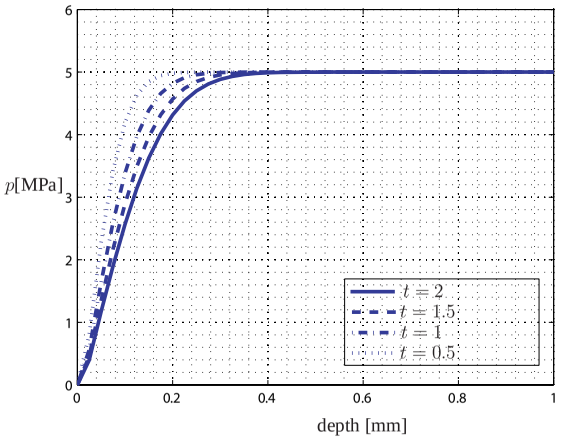
The material parameters are taken like the consolidation problem from table 4.1. The mixed hybrid finite element uses the non-uniform grid which is more refined near



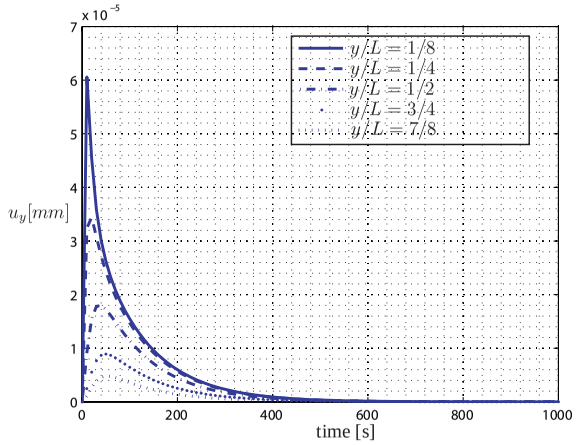
(a) Schematic representation of the consolidation problem.



(b) Analytical-MHFEM comparison of the displacement.



(c) MHFEM solution for fluid pressure at $y = L$.



(d) MHFEM solution for fluid flow.

Figure 4.4. Analytical-MHFEM comparison of the displacement, fluid pressure and fluid flow for the consolidation problem.

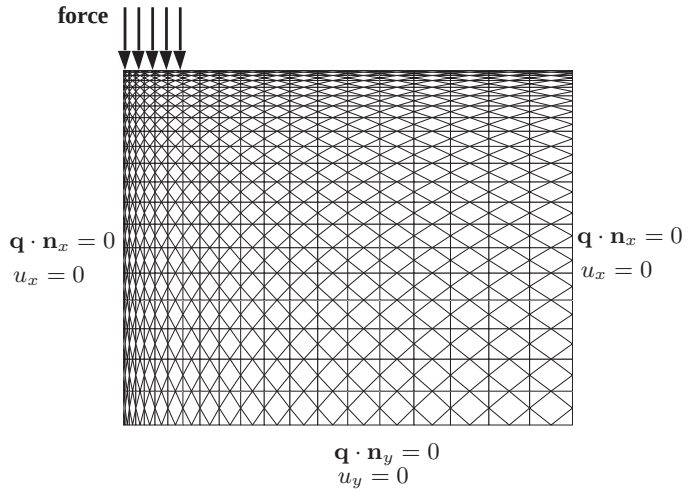


Figure 4.5. Mixed finite element mesh for the footing problem.

the upper left part. This problem is described in detail for the elastic consolidation problem in (Murad and Loula, 1994). The described geometry with the boundary conditions are described in Figure 4.5. The numerical results for the fluid pressure at different times are shown in Figure 4.6.

In the mixed formulation the flow is calculated as a primary variable, therefore the approximation of no-flow at the boundaries is more accurate than the Galerkin method. In fact, in the Galerkin method flows are calculated from fluid pressure and the displacement as secondary variables.

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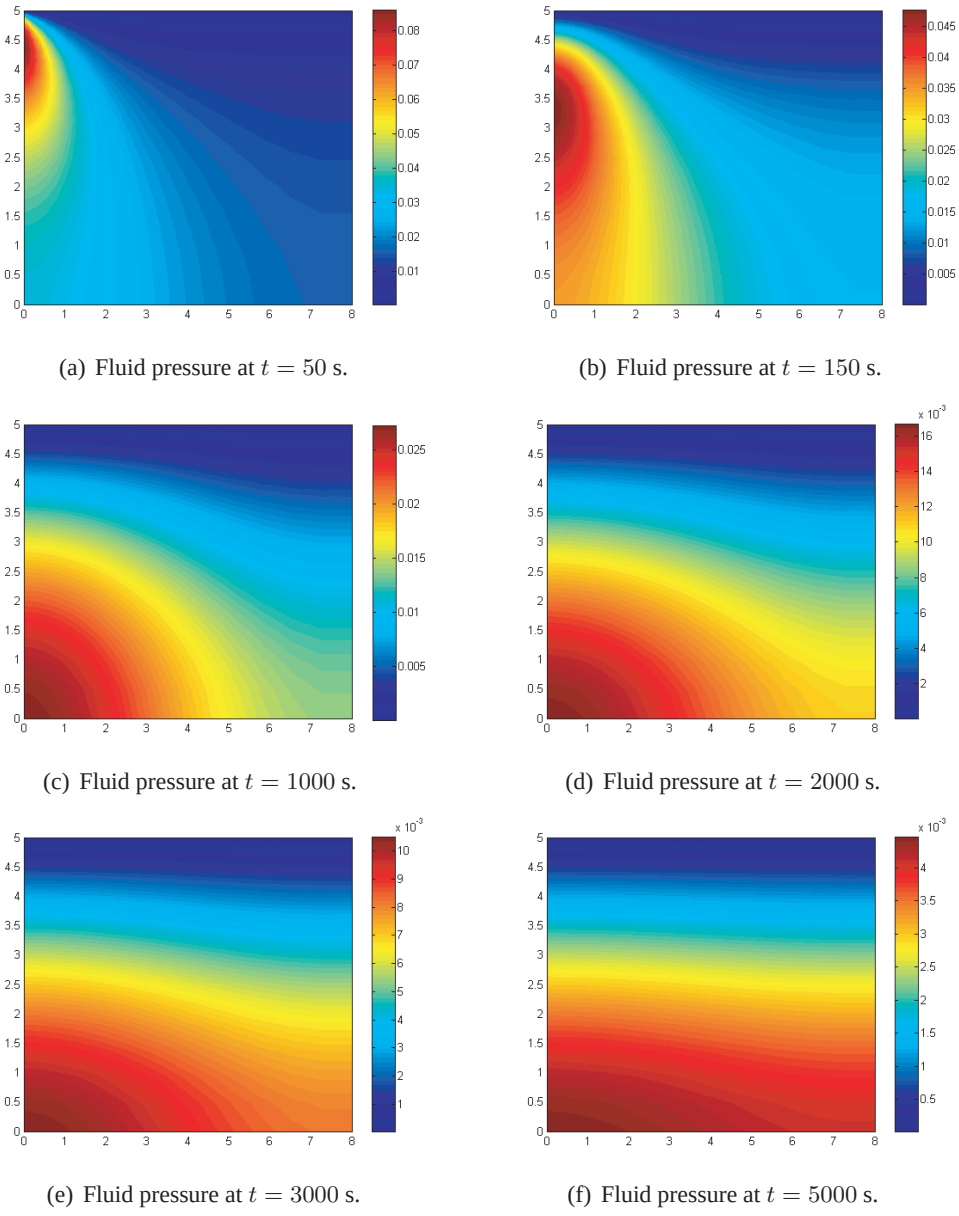


(a) Fluid pressure at $t = 50$ s.

(b) Fluid pressure at $t = 150$ s.

(c) Fluid pressure at $t = 1000$ s.

(d) Fluid pressure at $t = 2000$ s.

(e) Fluid pressure at $t = 3000$ s.

(f) Fluid pressure at $t = 5000$ s.

Figure 4.6. MHFEM solution for the fluid pressure of footing problem.

Chapter 5

Mixed and hybrid finite element solution for* four-component

In the previous section we gave a detailed overview on the mixed formulation for the two-component model. The solid-fluid interactions cannot describe the osmotic effects, which have a major influence on the behaviour of tissues. Therefore the objective of this chapter is to study the mixed variational formulation to derive a set of solutions for four-component model given in chapter 2.

Like the two-component model, also here it is desirable to obtain approximations of the fluid flow and ions flow that fulfil the conservation equations.

In finite element simulation (van Loon et al., 2003), (Ehlers et al., 2005a), (Ehlers et al., 2005b) and (Ehlers et al., 2006) these quantities are computed by differentiation of the electro-chemical potential solutions. This approach may lead to violation of the mass conservation principle.

The mixed finite element method provides an attractive framework for this type of problems by simultaneously approximating flows and electro-chemical potentials. Flows computed by mixed finite elements automatically satisfy the "divergence free" property, both locally and globally, and the corresponding normal flux field is guaranteed to be continuous across inter-element boundaries. The mixed finite element method has been extensively used for the solution of parabolic equations arising in different application fields. The mixed finite element method was proposed for two-dimensional problems by (Raviart and Thomas, 1977), (Thomas, 1977) and (Roberts and Thomas, 1991), and by Nédélec for three-dimensional problems (Nédélec, 1980) and (Nédélec, 1986). In this article the mixed finite element variational formulation is derived for the set of coupled equations in general dimensions. Only the lowest-order mixed method will be considered, first, because higher order-methods result in some conceptual complications and, second, because the lowest-order method is comparatively easy and straightforward to use for practical problems.

In steady-state flow problems, i.e., elliptic equations, the system derived from mixed formulation becomes indefinite. A common solution method discussed in the

* Parts of this chapter will be appeared in ESAIM: Mathematical Modelling and Numerical Analysis (Malakpoor et al., 2006b)

previous chapter is the so-called mixed-hybrid finite element (MHFEM) technique. Through the definition of an extra variable representing the pressure at element edges, MHFEM gives rise to a symmetric positive definite matrix with good conditioning properties. Using the MHFEM technique for our model, we still have an indefinite system but the advantage is that the number of degrees of freedom will be reduced. In fact, for a three-dimensional problem this number will be reduced from 15 to 6 degrees of freedom. Note that in our case the equations are time dependent and nonlinear, therefore a choice for time integration and a nonlinear solver is needed. We use some techniques to tackle this problem. In chapter 3 analytical solutions are given for linearised problem. Finally the results are validated for confined consolidation and free swelling experiments using the analytical solution.

5.1 The coupled mixed formulation

Remember that,

1. In four-component mixture theory a deformable and charged porous medium is saturated with a fluid with dissolved cations and anions.
2. The solid skeleton and fluid are assume to be intrinsically incompressible.
3. We assume that no chemical reactions exist between phases and no sources or sinks exist.
4. We neglect the inertia effects and body forces.
5. The materials are assumed to be isothermal.
6. The mixture is assumed to be saturated, i.e., (2.2.1) holds.
7. It is assumed that the solid matrix is entirely elastic and initially isotropic.
8. We assume infinitesimal deformation for the solid phase.

Let Ω be an open domain in $\mathbb{R}^n$, $n = 1, 2, 3$. Define $\Omega_T = \Omega \times (0, T]$ for $T > 0$, and consider the sets $\Gamma^D_{\mathbf{u}}$ and $\Gamma^N_{\mathbf{u}}$ (and similarly Γ^D_p and Γ^N_p) to be two disjoint open subsets of the total boundary $\Gamma = \partial\Omega$, such that $\Gamma^D_\alpha \cap \Gamma^N_\alpha = \emptyset$ and $\bar{\Gamma}^D_\alpha \cup \bar{\Gamma}^N_\alpha = \Gamma$ for $\alpha = \mathbf{u}$ and p. We assume meas $\Gamma^D_\alpha > 0$ for $\alpha = \mathbf{u}, p$.

Remember the definitions of the spaces $H^D_1(\Omega)$, $\mathcal{V}$ and $H_N(\mathrm{div}; \Omega)$ in section 4.1:

$$
\begin{aligned}
\mathcal{V} &= \left\{\mathbf{u} \in (H^1(\Omega))^n : \mathbf{u} = 0 \text{ on } \Gamma^D_{\mathbf{u}}\right\} \\
H^1_D(\Omega) &= \left\{\varphi \in H^1(\Omega) : \varphi = 0 \text{ on } \Gamma^D_p\right\}, \\
H_N(\mathrm{div}; \Omega) &= \left\{\mathbf{q} \in H(\mathrm{div}; \Omega) : \mathbf{n} \cdot \mathbf{q} = 0 \text{ on } \Gamma^N_p\right\}, \\
H^{-1/2}_N(\Gamma) &= \left\{\mu \in H^{-1/2}(\Gamma) : \mu = 0 \text{ on } \Gamma^N_p\right\}.
\end{aligned}
$$

The total set of equations describing the four-component model is given in (2.7.7):

		Conservation Equations	
$\mathbf{0}$	$=$	$\nabla \cdot \boldsymbol{\sigma} - \nabla p,$	
0	$=$	$\dfrac{\partial \nabla \cdot \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{q}^l,$	
0	$=$	$\dfrac{\partial (\nabla \cdot \mathbf{u} + \varphi_0) c^\beta}{\partial t} + \nabla \cdot (\mathbf{q}^\beta + c^\beta \mathbf{q}^l), \quad \beta = +, -,$	
		Constitutive Equations	
$\boldsymbol{\sigma}$	$=$	$2\mu_s \boldsymbol{\mathcal{E}} + \lambda_s \mathrm{tr}\boldsymbol{\mathcal{E}}, \quad \boldsymbol{\mathcal{E}} = \dfrac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u}^T)),$	
$\mathbf{q}^l$	$=$	$-K(\nabla \mu^l + c^+ \nabla \mu^+ + c^- \nabla \mu^-),$	
$\mathbf{q}^\beta$	$=$	$-\dfrac{D^\beta}{RT} \varphi c^\beta \nabla \mu^\beta, \quad \beta = +, -,$	
		Secondary Equations	
φ	$=$	$1 - (1 - \varphi_0)(1 - \nabla \cdot \mathbf{u})$	
c^{fc}	$=$	$c_0^{fc} \left(1 - \dfrac{\nabla \cdot \mathbf{u}}{\varphi_0}\right)$	
c^β	$=$	$-\dfrac{1}{2z^\beta} z^{fc} c^{fc} +$	
	$+$	$\dfrac{1}{2}\sqrt{(z^{fc} c^{fc})^2 + \dfrac{4c^2}{f^+ f^-} \exp \dfrac{\mu^+ - \mu_0^+ + \mu^- - \mu_0^-}{RT}},$	
p	$=$	$\mu^l - \mu_0^l + RT\left(\Gamma^+ c^+ + \Gamma^- c^-\right),$	
ξ	$=$	$\dfrac{1}{z^\beta F}\left(\mu^\beta - \mu_0^\beta - RT \ln \dfrac{f^\beta c^\beta}{c}\right), \quad \beta = +, -,$	
		Boundary Conditions	
$\mathbf{u}$	$=$	$\mathbf{0}$	on $\Gamma_{\mathbf{u}}^D \times (0, T],$
μ^l	$=$	μ_{in}^l	on $\Gamma_p^D \times (0, T],$
μ^+	$=$	μ_{in}^+	on $\Gamma_p^D \times (0, T],$
μ^-	$=$	μ_{in}^-	on $\Gamma_p^D \times (0, T],$
$\mathbf{g}_{\mathbf{u}}^N$	$=$	$\mathbf{n} \cdot (\boldsymbol{\sigma}(\mathbf{u}) - p)$	on $\Gamma_{\mathbf{u}}^N \times (0, T],$
$\mathbf{n} \cdot \mathbf{q}^l$	$=$	0	on $\Gamma_p^N \times (0, T],$
$\mathbf{n} \cdot \mathbf{q}^+$	$=$	0	on $\Gamma_p^N \times (0, T],$
$\mathbf{n} \cdot \mathbf{q}^-$	$=$	0	on $\Gamma_p^N \times (0, T].$

For the preliminary step of defining a spatially semi-discrete approximate solution to our initial boundary value problem, we write the problem in weak form. We introduce a mixed variational formulation of the problem with the related boundary conditions. Define $\mathbf{q}_{\mathrm{tot}}^\beta = \mathbf{q}^\beta + c^\beta \mathbf{q}^l$ for $\beta = +, -$. Then the mixed variation formulation of the

problem reads:

$$\begin{cases} \displaystyle\int_\Omega \left(2\mu_s \boldsymbol{\mathcal{E}}(\mathbf{u}) : \boldsymbol{\mathcal{E}}(\bar{\mathbf{u}}) + \lambda_s \nabla\cdot\mathbf{u}\nabla\cdot\bar{\mathbf{u}}\right)\, d\mathbf{x} - \int_\Omega \mu^l \nabla\cdot\bar{\mathbf{u}}\, d\mathbf{x} = \\ \displaystyle\int_\Omega \Big(RT(\Gamma^+c^+ + \Gamma^-c^-) - \mu_0^l - p_{in}\Big)\nabla\cdot\bar{\mathbf{u}}\, d\mathbf{x} + \int_{\Gamma_{\mathbf{u}}^N} \mathbf{g}_{\mathbf{u}}^N\cdot\bar{\mathbf{u}}\, ds, & (5.1.1a) \\ \displaystyle\frac{1}{K}\int_\Omega \mathbf{q}^l\cdot\bar{\mathbf{q}}^l\, d\mathbf{x} + \int_\Omega \nabla\mu^l\cdot\bar{\mathbf{q}}^l\, d\mathbf{x} + \sum_{\beta=+,-}\int_\Omega c^\beta\nabla\mu^\beta\cdot\bar{\mathbf{q}}^l\, d\mathbf{x} = 0, & (5.1.1b) \\ \displaystyle\frac{RT}{D^\beta}\int_\Omega \mathbf{q}^\beta\cdot\bar{\mathbf{q}}^\beta\, d\mathbf{x} + \int_\Omega \nabla\mu^\beta\cdot\bar{\mathbf{q}}^\beta\, d\mathbf{x} = 0,\ \beta = +,-, & (5.1.1c) \\ \displaystyle -\int_\Omega \nabla\cdot\mathbf{q}^l\bar{\mu}^l\, d\mathbf{x} - \int_\Omega \frac{\partial\nabla\cdot\mathbf{u}}{\partial t}\bar{\mu}^l\, d\mathbf{x} = 0, & (5.1.1d) \\ \displaystyle -\int_\Omega \nabla\cdot\mathbf{q}_{\mathrm{tot}}^\beta\bar{\mu}^\beta\, d\mathbf{x} = \int_\Omega \frac{\partial(\nabla\cdot\mathbf{u}+\varphi_0)c^\beta}{\partial t}\bar{\mu}^\beta\, d\mathbf{x},\ \beta = +,-, & (5.1.1e) \end{cases}$$

where $\bar{\mathbf{q}}^\beta = \bar{\mathbf{q}}_{\mathrm{tot}}^\beta - c^\beta\bar{\mathbf{q}}^l$.

Note that the solution is time dependent. After summing up equations (5.1.1b) and (5.1.1d), using the fact that $\bar{\mathbf{q}}_{\mathrm{tot}}^\beta$ is in $H_N(\mathrm{div};\Omega)$ and applying the Green's formula the above problem is rewritten as:

Find $\left(\mathbf{u}, \mathbf{q}^l, \mathbf{q}_{\mathrm{tot}}^+, \mathbf{q}_{\mathrm{tot}}^-, \mu^l, \mu^+, \mu^-\right)(\cdot,t) \in \mathcal{V}\times H_N(\mathrm{div};\Omega)\times H_N(\mathrm{div};\Omega)\times H_N(\mathrm{div};\Omega)\times L^2(\Omega)\times L^2(\Omega)\times L^2(\Omega)$, such that

$$\begin{cases} \displaystyle\int_\Omega \left(2\mu_s \boldsymbol{\mathcal{E}}(\mathbf{u}) : \boldsymbol{\mathcal{E}}(\bar{\mathbf{u}}) + \lambda_s \nabla\cdot\mathbf{u}\nabla\cdot\bar{\mathbf{u}}\right)\, d\mathbf{x} - \int_\Omega \mu^l \nabla\cdot\bar{\mathbf{u}}\, d\mathbf{x} = \\ \displaystyle\int_\Omega \Big(RT(\Gamma^+c^+ + \Gamma^-c^-) - \mu_0^l - p_{in}\Big)\nabla\cdot\bar{\mathbf{u}}\, d\mathbf{x} + \int_{\Gamma_{\mathbf{u}}^N} \mathbf{g}_{\mathbf{u}}^N\cdot\bar{\mathbf{u}}\, ds, & (5.1.2a) \\ \displaystyle\frac{1}{K}\int_\Omega \mathbf{q}^l\cdot\bar{\mathbf{q}}^l\, d\mathbf{x} + \sum_{\beta=+,-}\frac{RT}{D^\beta}\int_\Omega \frac{(\mathbf{q}_{\mathrm{tot}}^\beta - c^\beta\mathbf{q}^l)\cdot(\bar{\mathbf{q}}_{\mathrm{tot}}^\beta - c^\beta\bar{\mathbf{q}}^l)}{\varphi c^\beta}\, d\mathbf{x} \\ \displaystyle\quad -\int_\Omega \mu^l\nabla\cdot\bar{\mathbf{q}}^l\, d\mathbf{x} - \sum_{\beta=+,-}\int_\Omega \mu^\beta\nabla\cdot\bar{\mathbf{q}}_{\mathrm{tot}}^\beta\, d\mathbf{x} \\ \displaystyle = -\int_{\Gamma_p^D}\mu_{in}^l\mathbf{n}\cdot\bar{\mathbf{q}}^l\, ds - \sum_{\beta=+,-}\int_{\Gamma_p^D}\mu_{in}^\beta\mathbf{n}\cdot\bar{\mathbf{q}}_{\mathrm{tot}}^\beta\, ds, & (5.1.2b) \\ \displaystyle -\int_\Omega \nabla\cdot\mathbf{q}^l\bar{\mu}^l\, d\mathbf{x} - \int_\Omega \frac{\partial\nabla\cdot\mathbf{u}}{\partial t}\bar{\mu}^l\, d\mathbf{x} = 0, & (5.1.2c) \\ \displaystyle -\int_\Omega \nabla\cdot\mathbf{q}_{\mathrm{tot}}^\beta\bar{\mu}^\beta\, d\mathbf{x} = \int_\Omega \frac{\partial(\nabla\cdot\mathbf{u}+\varphi_0)c^\beta}{\partial t}\bar{\mu}^\beta\, d\mathbf{x},\ \beta = +,-, & (5.1.2d) \end{cases}$$

for all test functions $\left(\bar{\mathbf{u}}, \bar{\mathbf{q}}^l, \bar{\mathbf{q}}^+_{\rm tot}, \bar{\mathbf{q}}^-_{\rm tot}, \bar{\mu}^l, \bar{\mu}^+, \bar{\mu}^-\right) \in \mathcal{V}\times H_N(\mathrm{div};\Omega)\times H_N(\mathrm{div};\Omega)\times H_N(\mathrm{div};\Omega)\times L^2(\Omega)\times L^2(\Omega)\times L^2(\Omega)$ and $t>0$. Note that the solution is time dependent.

Denote the triple $(\mathbf{q}^l, \mathbf{q}^+_{\rm tot}, \mathbf{q}^-_{\rm tot})$ and (μ^l, μ^+, μ^-) by $\mathbf{q}$ and $\boldsymbol{\mu}$, respectively, and define:

$$
\begin{aligned}
a(\mathbf{u},\bar{\mathbf{u}}) &= \int_\Omega (2\mu_s \boldsymbol{\mathcal{E}}(\mathbf{u}) : \boldsymbol{\mathcal{E}}(\bar{\mathbf{u}}) + \lambda_s \nabla\cdot\mathbf{u}\nabla\cdot\bar{\mathbf{u}})\, d\mathbf{x},\\
b(\mathbf{u},\bar{\mu}^l) &= -\int_\Omega \nabla\cdot\mathbf{u}\bar{\mu}^l\, d\mathbf{x},\\
c(\mathbf{q},\bar{\mathbf{q}}) &= \frac{1}{K}\int_\Omega \mathbf{q}^l\cdot\bar{\mathbf{q}}^l\, d\mathbf{x} + \sum_{\beta=+,-}\frac{RT}{D^\beta}\int_\Omega \frac{(\mathbf{q}^\beta_{\rm tot}-c^\beta\mathbf{q}^l)\cdot(\bar{\mathbf{q}}^\beta_{\rm tot}-c^\beta\bar{\mathbf{q}}^l)}{\varphi c^\beta}\, d\mathbf{x},\\
d^l(\mathbf{q}^l,\bar{\mu}^l) &= -\int_\Omega \nabla\cdot\mathbf{q}^l\bar{\mu}^l\, d\mathbf{x},\\
d^\beta(\mathbf{q}^\beta_{\rm tot},\bar{\mu}^\beta) &= -\int_\Omega \nabla\cdot\mathbf{q}^\beta_{\rm tot}\bar{\mu}^\beta\, d\mathbf{x},\quad \beta=+,-,\\
F(\bar{\mathbf{u}}) &= \int_\Omega \Big(RT(\Gamma^+c^+ + \Gamma^-c^-) - \mu^l_0 - p_{in}\Big)\nabla\cdot\bar{\mathbf{u}}\, d\mathbf{x} + \int_{\Gamma^N_{\mathbf{u}}} \mathbf{g}^N_{\mathbf{u}}\cdot\bar{\mathbf{u}}\, ds,\\
F_1(\bar{\mathbf{q}}) &= -\int_{\Gamma^D_p}\mu^l_{in}\mathbf{n}\cdot\bar{\mathbf{q}}^l - \sum_{\beta=+,-}\int_{\Gamma^D_p}\mu^\beta_{in}\mathbf{n}\cdot\bar{\mathbf{q}}^\beta_{\rm tot}\, ds,\\
F_2^\beta(\bar{\mu}^\beta) &= \int_\Omega(\nabla\cdot\mathbf{u}+\varphi_0)c^\beta\bar{\mu}^\beta\, d\mathbf{x},\quad \beta=+,-,
\end{aligned}
$$

then the problem (5.1.2a) - (5.1.2d) can be rewritten as follows:

Find $\left(\mathbf{u}, \mathbf{q}^l, \mathbf{q}^+_{\rm tot}, \mathbf{q}^-_{\rm tot}, \mu^l, \mu^+, \mu^-\right) \in \mathcal{V}\times H_N(\mathrm{div};\Omega)\times H_N(\mathrm{div};\Omega)\times H_N(\mathrm{div};\Omega)\times L^2(\Omega)\times L^2(\Omega)\times L^2(\Omega)$ such that

$$
\begin{array}{lllll}
a(\mathbf{u},\bar{\mathbf{u}}) & & +b(\bar{\mathbf{u}},\mu^l) & & = F(\bar{\mathbf{u}}),\\
 & c(\mathbf{q},\bar{\mathbf{q}}) & +d^l(\bar{\mathbf{q}}^l,\mu^l)+d^+(\bar{\mathbf{q}}^+_{\rm tot},\mu^+)+d^-(\bar{\mathbf{q}}^-_{\rm tot},\mu^-) & & = F_1(\bar{\mathbf{q}}),\\
\dfrac{d}{dt}b(\mathbf{u},\bar{\mu}^l) & +d^l(\mathbf{q}^l,\bar{\mu}^l) & & & = 0,\\
 & d^+(\mathbf{q}^+_{\rm tot},\bar{\mu}^+) & & & = \dfrac{d}{dt}F_2^+(\bar{\mu}^+),\\
 & d^-(\mathbf{q}^-_{\rm tot},\bar{\mu}^-) & & & = \dfrac{d}{dt}F_2^-(\bar{\mu}^-),
\end{array}
\tag{5.1.3}
$$

for all test functions $\left(\bar{\mathbf{u}}, \bar{\mathbf{q}}^l, \bar{\mathbf{q}}^+_{\rm tot}, \bar{\mathbf{q}}^-_{\rm tot}, \bar{\mu}^l, \bar{\mu}^+, \bar{\mu}^-\right) \in \mathcal{V}\times H_N(\mathrm{div};\Omega)\times H_N(\mathrm{div};\Omega)\times H_N(\mathrm{div};\Omega)\times L^2(\Omega)\times L^2(\Omega)\times L^2(\Omega)$ and $t>0$.

We shall use the implicit Euler scheme for time discretisation. Let Δt be the time step and $\left(\mathbf{u}_n, \mathbf{q}^l_n, \mathbf{q}^+_{{\rm tot},n}, \mathbf{q}^-_{{\rm tot},n}, \mu^l_n, \mu^+_n, \mu^-_n\right)$ the approximation of the solution vector $\left(\mathbf{u}, \mathbf{q}^l, \mathbf{q}^+_{\rm tot}, \mathbf{q}^-_{\rm tot}, \mu^l, \mu^+, \mu^-\right)$ at $t=t_n=n\Delta t$. Then the system of equation (5.1.3) resulting from backward Euler is:

Find $\left(\mathbf{u}_n, \mathbf{q}_n^l, \mathbf{q}_{\text{tot},n}^+, \mathbf{q}_{\text{tot},n}^-, \mu_n^l, \mu_n^+, \mu_n^-\right) \in \mathcal{V} \times H_N(\text{div};\Omega) \times H_N(\text{div};\Omega)$
$\times H_N(\text{div};\Omega) \times L^2(\Omega) \times L^2(\Omega) \times L^2(\Omega)$ such that

$$\begin{array}{lllll} a(\mathbf{u}_n, \bar{\mathbf{u}}) & & +b(\bar{\mathbf{u}}, \mu_n^l) & = & F_n(\bar{\mathbf{u}}), \\ & \Delta tc_n(\mathbf{q}_n, \bar{\mathbf{q}}) & +\Delta td^l(\bar{\mathbf{q}}^l, \mu_n^l)+\Delta td^+(\bar{\mathbf{q}}_{\text{tot}}^+, \mu_n^+)+\Delta td^-(\bar{\mathbf{q}}_{\text{tot}}^-, \mu_n^-) & = & \Delta tF_{1,n}(\bar{\mathbf{q}}), \\ b(\mathbf{u}_n, \bar{\mu}^l) & +\Delta td^l(\mathbf{q}_n^l, \bar{\mu}^l) & & = & b(\mathbf{u}_{n-1}, \bar{\mu}^l), \\ & \Delta td^+(\mathbf{q}_{\text{tot},n}^+, \bar{\mu}^+) & & = & \mathcal{F}_{2,n}^+(\bar{\mu}^+), \\ & \Delta td^-(\mathbf{q}_{\text{tot},n}^-, \bar{\mu}^-) & & = & \mathcal{F}_{2,n}^-(\bar{\mu}^-), \end{array} \tag{5.1.4}$$

for all test functions $\left(\bar{\mathbf{u}}, \bar{\mathbf{q}}^l, \bar{\mathbf{q}}_{\text{tot}}^+, \bar{\mathbf{q}}_{\text{tot}}^-, \bar{\mu}^l, \bar{\mu}^+, \bar{\mu}^-\right) \in \mathcal{V} \times H_N(\text{div};\Omega) \times H_N(\text{div};\Omega) \times H_N(\text{div};\Omega) \times L^2(\Omega) \times L^2(\Omega) \times L^2(\Omega)$, where

$$\mathcal{F}_n^\beta(\bar{\mu}^\beta) = F_{2,n}^\beta(\bar{\mu}^\beta) - F_{2,n-1}^\beta(\bar{\mu}^\beta), \quad \beta = +, -.$$

where

$$F_{2,n}^\beta(\bar{\mu}^\beta) = \int_\Omega \left(\nabla \cdot \mathbf{u}_n + \varphi_0\right) c_n^\beta \bar{\mu}^\beta \, d\mathbf{x}, \quad \beta = +, -.$$

Note that the dependency of $c_n(\mathbf{q}_n, \bar{\mathbf{q}})$, $F_n(\bar{\mathbf{u}})$, $F_{1,n}(\bar{\mathbf{q}})$ and $\mathcal{F}_{2,n}^\beta(\bar{\mu}^+)$ to n is because of φ_n and c_n^β. Note that also we need some iteratie procedure to solve the nonlinear system of equations. Let us define two forms

$$\begin{aligned} \mathbb{A}_n(\mathbf{u}, \mathbf{q}; \bar{\mathbf{u}}, \bar{\mathbf{q}}) &= a(\mathbf{u}, \bar{\mathbf{u}}) + \Delta tc_n(\mathbf{q}, \bar{\mathbf{q}}), & (5.1.5) \\ \mathbb{B}(\mathbf{u}, \mathbf{q}; \bar{\boldsymbol{\mu}}) &= b(\mathbf{u}, \bar{\mu}^l) + \Delta td^l(\mathbf{q}^l, \bar{\mu}^l) + \Delta td^+(\mathbf{q}_{\text{tot}}^+, \bar{\mu}^+) \\ &+ \Delta td^-(\mathbf{q}_{\text{tot}}^-, \bar{\mu}^-), & (5.1.6) \end{aligned}$$

and forms

$$\begin{aligned} G_{1,n}(\bar{\mathbf{u}}, \bar{\mathbf{q}}) &= \left(F_n(\bar{\mathbf{u}}), \Delta tF_{1,n}(\bar{\mathbf{q}})\right)^T, \\ G_{2,n}(\bar{\boldsymbol{\mu}}) &= \left(b(\mathbf{u}_{n-1}, \bar{\mu}^l), \mathcal{F}_n^+(\bar{\mu}^+), \mathcal{F}_n^-(\bar{\mu}^-)\right)^T, \end{aligned}$$

then (5.1.4) is rewritten as

$$\begin{array}{l} \text{Find } (\mathbf{u}_n, \mathbf{q}_n, \boldsymbol{\mu}_n) \in \mathcal{V} \times (H_N(\text{div};\Omega))^3 \times (L^2(\Omega))^3 \\ \\ \begin{array}{ll} \mathbb{A}_n(\mathbf{u}_n, \mathbf{q}_n; \bar{\mathbf{u}}, \bar{\mathbf{q}}) + \mathbb{B}(\bar{\mathbf{u}}, \bar{\mathbf{q}}; \boldsymbol{\mu}_n) & = G_{1,n}(\bar{\mathbf{u}}), \\ \mathbb{B}(\mathbf{u}_n, \mathbf{q}_n; \bar{\boldsymbol{\mu}}) & = G_{2,n}(\bar{\boldsymbol{\mu}}), \end{array} \end{array} \tag{5.1.7}$$

for all test functions $(\bar{\mathbf{u}}, \bar{\mathbf{q}}, \bar{\boldsymbol{\mu}}) \in \mathcal{V} \times (H_N(\text{div};\Omega))^3 \times (L^2(\Omega))^3$.

As we can see the mixed variational formulation of the four-component model also can be written as a saddle point problem but the main difference between this system and the system in (4.2.6) is that here the bilinear forms are function of φ, c^+ and c^-.

Let skip the subscript n in the above system and assume that φ, c^+ and c^- are given, then we have the following theorem:

Theorem 5.1. *Consider the saddle point problem* (5.1.7)*. Assume that φ, c^+ and c^- are given, then*

(i) The bilinear form $\mathbb{A}$ is $\ker(\mathbb{B})$-elliptic, i.e., there exists a positive constant $\alpha(\varphi, c^+, c^-)$ such that

$$\mathbb{A}(\mathbf{u}, \mathbf{q}; \mathbf{u}, \mathbf{q}) \geq \alpha \, |||(\mathbf{u}, \mathbf{q})|||_1, \quad \textit{for all } (\mathbf{u}, \mathbf{q}) \in \ker(\mathbb{B}).$$

where

$$|||(\mathbf{u}, \mathbf{q})|||_1 = \left(\|\mathbf{u}\|_1^2 + \|\mathbf{q}^l\|_{\mathrm{div};\Omega}^2 + \|\mathbf{q}_{\mathrm{tot}}^+\|_{\mathrm{div};\Omega}^2 + \|\mathbf{q}_{\mathrm{tot}}^-\|_{\mathrm{div};\Omega}^2 \right)^{1/2}.$$

(ii) The bilinear $\mathbb{B}$ satisfies the inf-sup condition

$$\sup_{\mathbf{q} \in (H_N(div;\Omega))^3} \frac{\mathbb{B}(\mathbf{u}, \mathbf{q}; \boldsymbol{\mu})}{|||(\mathbf{u}, \mathbf{q})|||_1} \geq \beta \|\boldsymbol{\mu}\|_0 \quad \textit{for all } \boldsymbol{\mu} \in (L^2(\Omega))^3.$$

Proof. To prove the first part, we follow the proof in (4.2.14). Take $(\mathbf{u}, \mathbf{q}) \in \ker(\mathbb{B})$, then we have

$$\int_\Omega \nabla \cdot \mathbf{u} \bar{\mu}^l \, d\mathbf{x} + \Delta t \left(\int_\Omega \nabla \cdot \mathbf{q}^l \bar{\mu}^l \, d\mathbf{x} + \int_\Omega \nabla \cdot \mathbf{q}_{\mathrm{tot}}^+ \bar{\mu}^+ \, d\mathbf{x} + \int_\Omega \nabla \cdot \mathbf{q}_{\mathrm{tot}}^- \bar{\mu}^- \, d\mathbf{x} \right) = 0,$$

for all $\bar{\boldsymbol{\mu}} = (\bar{\mu}^l, \bar{\mu}^+, \bar{\mu}^-) \in (L^2(\Omega))^3$. This results into

$$\nabla \cdot \mathbf{u} + \Delta t \nabla \cdot \mathbf{q}^l = 0, \tag{5.1.8}$$

$$\nabla \cdot \mathbf{q}_{\mathrm{tot}}^+ = 0, \tag{5.1.9}$$

$$\nabla \cdot \mathbf{q}_{\mathrm{tot}}^- = 0. \tag{5.1.10}$$

It is easy to see that

$$c(\mathbf{q}, \bar{\mathbf{q}}) = \int_\Omega \mathbf{q} \mathbf{C}^{l\pm} \bar{\mathbf{q}} \, d\mathbf{x}, \tag{5.1.11}$$

where

$$\mathbf{C}^{l\pm} = \begin{pmatrix} \frac{1}{K} + \frac{RTc^+}{D^+\varphi} + \frac{RTc^-}{D^-\varphi} & -\frac{RT}{D^+\varphi} & -\frac{RT}{D^-\varphi} \\ -\frac{RT}{D^+\varphi} & \frac{RT}{D^+\varphi c^+} & 0 \\ -\frac{RT}{D^-\varphi} & 0 & \frac{RT}{D^-\varphi c^-} \end{pmatrix}. \tag{5.1.12}$$

But $\mathbf{C}^{l\pm}$ is symmetric positive definite. Indeed, if we define $\mathbf{N} = \mathrm{diag}\,(1, c^+, c^-)$, then we have

$$\varphi^2 \mathbf{N} \mathbf{C}^{l\pm} \mathbf{N} = \begin{pmatrix} \frac{\varphi^2}{K} + \frac{RTc^+\varphi}{D^+} + \frac{RTc^-\varphi}{D^-} & -\frac{RTc^+\varphi}{D^+} & -\frac{RTc^-\varphi}{D^-} \\ -\frac{RTc^+\varphi}{D^+} & \frac{RTc^+\varphi}{D^+} & 0 \\ -\frac{RTc^-\varphi}{D^-} & 0 & \frac{RTc^-\varphi}{D^-} \end{pmatrix}.$$

In Lemma 3.2 we proved that this matrix is symmetric positive definite.

Now let us continue the proof of $\ker(\mathbb{B})$-ellipticity of the bilinear form $\mathbb{A}$. Take $(\mathbf{u},\mathbf{q}) \in \ker(\mathbb{B})$, then by using Korn's inequality (4.2.12) and equations (5.1.8) - (5.1.11) we have

$$\begin{aligned}
&\mathbb{A}(\mathbf{u},\mathbf{q};\mathbf{u},\mathbf{q}) = a(\mathbf{u},\mathbf{u}) + \Delta t c(\mathbf{q},\mathbf{q}) \\
= &\int_\Omega 2\mu_s \boldsymbol{\mathcal{E}}(\mathbf{u}) : \boldsymbol{\mathcal{E}}(\mathbf{u}) + \lambda_s(\nabla\cdot\mathbf{u})^2\, d\mathbf{x} + \Delta t \int_\Omega (\mathbf{q}^l, \mathbf{q}^+_{\rm tot}, \mathbf{q}^-_{\rm tot})\mathbf{C}^{l\pm} \begin{pmatrix} \bar{\mathbf{q}}^l \\ \bar{\mathbf{q}}^+_{\rm tot} \\ \bar{\mathbf{q}}^-_{\rm tot} \end{pmatrix} \\
\geq\ & 2\mu_s c\|\mathbf{u}\|_1^2 + \lambda_s\|\nabla\cdot\mathbf{u}\|_0^2 + C\Delta t(\|\mathbf{q}^l\|_0^2 + \|\mathbf{q}^+_{\rm tot}\|_0^2 + \|\mathbf{q}^-_{\rm tot}\|_0^2) \\
\geq\ & 2\mu_s c\|\mathbf{u}\|_1^2 + \lambda_s(\Delta t)^2\|\nabla\cdot\mathbf{q}^l\|_0^2 + C\Delta t(\|\mathbf{q}^l\|_0^2 + \|\mathbf{q}^+_{\rm tot}\|^2_{{\rm div};\Omega} + \|\mathbf{q}^-_{\rm tot}\|^2_{{\rm div};\Omega}) \\
\geq\ & \alpha\, |||\,(\mathbf{u},\mathbf{q})|||_1, \qquad (5.1.13)
\end{aligned}$$

where $\alpha = \min(2\mu_s c, \lambda_s(\Delta t)^2, C)$ and $C = C(\varphi, c^+, c^-)$.
To prove the second part (inf-sup condition), we restrict the supremum to a subset of functions $(\mathbf{0},\mathbf{q})$,

$$\Delta t \sup_{\mathbf{q}\in(H_N({\rm div};\Omega))^3} \frac{d^l(\mathbf{q}^{\mathbf{l}},\mu^l) + d^+(\mathbf{q}^+_{\rm tot},\mu^+) + d^-(\mathbf{q}^-_{\rm tot}\mu^-)}{\|\mathbf{q}\|_{{\rm div};\Omega}} \geq \tilde{\beta}\|\boldsymbol{\mu}\|_0,$$

for all $\boldsymbol{\mu} \in (L^2(\Omega))^3$. Easily it can be seen that the above supremum is greater or equal than

$$\begin{aligned}
\Delta t \sup_{\mathbf{q}^l\in H_N({\rm div};\Omega)} \frac{d^l(\mathbf{q}^{\mathbf{l}},\mu^l)}{\|\mathbf{q}^l\|_{{\rm div};\Omega}} \quad &+ \quad \sup_{\mathbf{q}^+_{\rm tot}\in H_N({\rm div};\Omega)} \frac{d^+(\mathbf{q}^+_{\rm tot},\mu^+)}{\|\mathbf{q}^+_{\rm tot}\|_{{\rm div};\Omega}} \\
&+ \quad \sup_{\mathbf{q}^-_{\rm tot}\in H_N({\rm div};\Omega)} \frac{d^-(\mathbf{q}^-_{\rm tot},\mu^-)}{\|\mathbf{q}^-_{\rm tot}\|_{{\rm div};\Omega}}.
\end{aligned}$$

In fact, we split the inf-sup condition to three inf-sup condition for each component, liquid, cation and anion. Following the proof for Theorem 4.4, we have a lower bound for each of the above terms, therefore

$$\begin{aligned}
&\Delta t \sup_{\mathbf{q}\in(H_N({\rm div};\Omega))^3} \frac{d^l(\mathbf{q}^{\mathbf{l}},\mu^l) + d^+(\mathbf{q}^+_{\rm tot},\mu^+) + d^-(\mathbf{q}^-_{\rm tot},\mu^-)}{\|\mathbf{q}\|_{{\rm div};\Omega}} \\
\geq\ & \tilde{\beta}^l\|\mu^l\|_0 + \tilde{\beta}^+\|\mu^+\|_0 + \tilde{\beta}^-\|\mu^-\|_0 \\
\geq\ & \tilde{\beta}\left(\|\mu^l\|_0^2 + \|\mu^+\|_0^2 + \|\mu^-\|_0^2\right)^{1/2} \\
=\ & \tilde{\beta}\|\boldsymbol{\mu}\|_0. \qquad (5.1.14)
\end{aligned}$$

Therefore the inf-sup condition holds for all $\beta \leq \tilde{\beta}$. This proves the second part of the theorem. ■

Remark 5.2. *Following the above theorem, we can conclude that given φ, c^+ and c^- the solution for the system* (5.1.7) *exists and is unique. Moreover, one has the bounds*

$$|||\,(\mathbf{u},\mathbf{q})|||_1 \leq \frac{1}{\alpha}\|F\|_{-1} + \left(1+\frac{\|\mathbb{A}\|}{\alpha}\right)\frac{1}{\beta}\|G\|_{-1}, \tag{5.1.15}$$

$$\|\boldsymbol{\mu}\|_{(L^2(\Omega))^3\backslash\ker(\mathbb{B}^*)} \leq \frac{1}{\beta}\left(1+\frac{\|\mathbb{A}\|}{\alpha}\right)\|F\|_{-1} + \frac{\|\mathbb{A}\|}{\beta^2}\left(1+\frac{\|\mathbb{A}\|}{\alpha}\right)\|G\|_{-1}, \tag{5.1.16}$$

where

$$\ker(\mathbb{B}^*) = \left\{\boldsymbol{\mu}\in\mathbf{L}^2(\Omega)\,|\,\mathbb{B}(\mathbf{u},\mathbf{q};\boldsymbol{\mu}) = 0 \quad \textit{for all } (\mathbf{u},\mathbf{q})\in\mathcal{V}\times H_N(\mathrm{div};\Omega)\right\}.$$

5.2 Hybridization of the mixed method

In this section, hybridization technique is used for the four-component model. We introduce a hybridization procedure for the mixed formulation. This will simplify the solution of the algebraic system that must be solved in the procedure. The idea behind hybridization is to relax the continuity requirement for the variables $\mathbf{q}^l$ and $\mathbf{q}^\beta_{\mathrm{tot}}$ across the internal edges. This will require to enlarge the Raviart-Thomas space in which $\mathbf{q}^l$ and $\mathbf{q}^\beta_{\mathrm{tot}}$ are sought and to introduce Lagrange multipliers to enforce the continuity of the normal component of $\mathbf{q}^l$ and $\mathbf{q}^\beta_{\mathrm{tot}}$ across the inter-element boundaries.

From the algebraic point of view, systems resulting from hybridization have often rather transparent sparsity structure. Thus, the hybridization can be considered as a specific matrix stretching technique

In chapter 4 in detail we discussed the hybridization technique for a linear time-dependent two-component model. Despite to the fact that four-component model is nonlinear, it can be considered as three copies of Darcy's problem introduced by $\mathbf{q}^l$ and $\mathbf{q}^\beta_{\mathrm{tot}}$.

Using hybridization technique we introduce three Lagrange multiplier to ensure the continuity of $\mathbf{q}^l$ and $\mathbf{q}^\beta_{\mathrm{tot}}$ across internal edges. As we have seen in the previous chapter the Hybridization technique will reduce the number of unknowns to the displacement vector and the Lagrange multiplier. In four-component model we expect to end-up with displacement and three Lagrange multipliers as unknowns. This section is devoted to this fact.

Define

$$\mathcal{E}_h^\partial = \{e\in\mathcal{E}_h : e\subset\Gamma\}. \tag{5.2.1}$$

We assume that Γ_p^D is the union of some $e\in\mathcal{E}_h^\partial$.

Let $\tilde{\mu}^l_{in}$ and $\tilde{\mu}^\beta_{in}$, both in $L^2(\Omega)$, be piecewise constant approximations of μ^l_{in} and

μ_{in}^{β}, such that

$$\int_e (\tilde{\mu}_{in}^{l} - \mu_{in}^{l})\, ds = 0 \quad \text{for all } e \in \mathcal{E}_h^{\partial},\ e \subset \Gamma_p^D, \tag{5.2.2}$$

$$\int_e (\tilde{\mu}_{in}^{\beta} - \mu_{in}^{\beta})\, ds = 0 \quad \text{for all } e \in \mathcal{E}_h^{\partial},\ e \subset \Gamma_p^D,\ \beta = +, -. \tag{5.2.3}$$

The hybrid formulation will make use of Lagrangian multipliers belonging to the space $L^2(\mathcal{E}_h)$ that is defined to be the product space

$$L^2(\mathcal{E}_h) = \prod_{T \in \mathcal{T}_h} L^2(\partial T). \tag{5.2.4}$$

Recall that $M^0(e)$, $e \in \mathcal{E}_h$, is the space of constant functions on e. Define the multiplier spaces

$$M_{-1}^0(\mathcal{E}_h) = \{\lambda = (\lambda_e)_{e \in \mathcal{E}_h} \in H^{1/2}(\bigcup_{e \in \mathcal{E}_h} e) : \lambda_e \in M^0(e) \text{ for all } e \in \mathcal{E}_h\}, \tag{5.2.5}$$

$$M_{-1,D}^0(\mathcal{E}_h) = \{\lambda \in M_{-1}^0(\mathcal{E}_h) : \lambda = 0 \quad \text{on} \quad \Gamma_p^D\}, \tag{5.2.6}$$

$$M_{-1,l}^0(\mathcal{E}_h) = \{\lambda \in M_{-1}^0(\mathcal{E}_h) : \lambda = \tilde{\mu}_{in}^{l} \quad \text{on} \quad \Gamma_p^D\}, \tag{5.2.7}$$

$$M_{-1,\beta}^0(\mathcal{E}_h) = \{\lambda \in M_{-1}^0(\mathcal{E}_h) : \lambda = \tilde{\mu}_{in}^{\beta} \quad \text{on} \quad \Gamma_p^D\},\ \beta = +, -. \tag{5.2.8}$$

The following lemma is an immediate consequence of the above definitions.

Lemma 5.3. *Suppose* $\mathbf{q} \in RT_{-1}^0(\mathcal{T}_h)$*, then* $\mathbf{q} \in RT_{0,N}^0(\mathcal{T}_h)$ *if, and only if,*

$$\sum_{T \in \mathcal{T}_h} \int_{\partial T} \lambda \mathbf{n}_T \cdot \mathbf{q}\, ds = 0 \quad \textit{for all } \lambda \in M_{-1,D}^0(\mathcal{E}_h).$$

Mixed hybrid variational problem

A spatial semi-discrete approximation by considering the hybridization technique is as follows.

Find $\left(\mathbf{u}_h, \mathbf{q}_h^l, \mathbf{q}_{\text{tot},h}^+, \mathbf{q}_{\text{tot},h}^-, \mu_h^l, \mu_h^+, \mu_h^-, \lambda_h^l, \lambda_h^+, \lambda_h^-\right)(\cdot, t) \in (P_D^1(\mathcal{T}_h))^n \times RT_{-1}^0(\mathcal{T}_h) \times RT_{-1}^0(\mathcal{T}_h) \times RT_{-1}^0(\mathcal{T}_h) \times M_{-1}^0(\mathcal{T}_h) \times M_{-1}^0(\mathcal{T}_h) \times M_{-1}^0(\mathcal{T}_h) \times M_{-1,l}^0(\mathcal{E}_h) \times M_{-1,+}^0(\mathcal{E}_h) \times M_{-1,-}^0(\mathcal{E}_h)$, such that

$$
\begin{cases}
\displaystyle\int_\Omega (2\mu_s \boldsymbol{\mathcal{E}}(\mathbf{u}_h) : \boldsymbol{\mathcal{E}}(\bar{\mathbf{u}}_h) + \lambda_s \nabla\cdot\mathbf{u}_h \nabla\cdot\bar{\mathbf{u}}_h)\, d\mathbf{x} - \int_\Omega \mu_h^l \nabla\cdot\bar{\mathbf{u}}_h\, d\mathbf{x} \\
\displaystyle= \int_\Omega \Big(RT(\Gamma^+ c_h^+ + \Gamma^- c_h^-) - \mu_0^l - p_{in} \Big) \nabla\cdot\bar{\mathbf{u}}_h\, d\mathbf{x} + \int_{\Gamma_{\mathbf{u}}^N} \mathbf{g}_{\mathbf{u}}^N \cdot \bar{\mathbf{u}}_h\, ds, \qquad (5.2.9a) \\
\displaystyle\frac{1}{K}\int_\Omega \mathbf{q}_h^l \cdot \bar{\mathbf{q}}_h^l\, d\mathbf{x} + \sum_{\beta=+,-} \frac{RT}{D^\beta} \int_\Omega \frac{(\mathbf{q}_{\mathrm{tot},h}^\beta - c_h^\beta \mathbf{q}_h^l)(\bar{\mathbf{q}}_{\mathrm{tot},h}^\beta - c_h^\beta \bar{\mathbf{q}}_h^l)}{\varphi_h c_h^\beta}\, d\mathbf{x} \\
\displaystyle- \sum_{T\in\mathcal{T}_h} \left(\int_T \mu_h^l \nabla\cdot\bar{\mathbf{q}}_h^l\, d\mathbf{x} - \int_{\partial T} \lambda_h^l \mathbf{n}_T \cdot \bar{\mathbf{q}}_h^l\, ds \right) \\
\displaystyle- \sum_{\beta=+,-} \left[\sum_{T\in\mathcal{T}_h} \left(\int_T \mu_h^\beta \nabla\cdot\bar{\mathbf{q}}_{\mathrm{tot},h}^\beta\, d\mathbf{x} - \int_{\partial T} \lambda_h^\beta \mathbf{n}_T \cdot \bar{\mathbf{q}}_{\mathrm{tot},h}^\beta\, ds \right) \right] = 0, \qquad (5.2.9b) \\
\displaystyle- \sum_{T\in\mathcal{T}_h} \int_T \nabla\cdot\mathbf{q}_h^l \bar{\mu}_h^l\, d\mathbf{x} - \int_\Omega \frac{\partial \nabla\cdot\mathbf{u}_h}{\partial t} \bar{\mu}_h^l\, d\mathbf{x} = 0, \qquad (5.2.9c) \\
\displaystyle- \sum_{T\in\mathcal{T}_h} \int_T \nabla\cdot\mathbf{q}_{\mathrm{tot},h}^\beta \bar{\mu}_h^\beta\, d\mathbf{x} = \int_\Omega \frac{\partial(\nabla\cdot\mathbf{u}_h + \varphi_0) c_h^\beta}{\partial t} \bar{\mu}_h^\beta\, d\mathbf{x}, \quad \beta = +,-, \qquad (5.2.9d) \\
\displaystyle\sum_{T\in\mathcal{T}_h} \int_{\partial T} \mathbf{n}_T \cdot \mathbf{q}_h^l \bar{\lambda}_h^l\, ds = 0, \qquad (5.2.9e) \\
\displaystyle\sum_{T\in\mathcal{T}_h} \int_{\partial T} \mathbf{n}_T \cdot \mathbf{q}_{\mathrm{tot},h}^\beta \bar{\lambda}_h^\beta\, ds = 0, \quad \beta = +,-, \qquad (5.2.9f)
\end{cases}
$$

for all test functions $\left(\bar{\mathbf{u}}_h, \bar{\mathbf{q}}_h^l, \bar{\mathbf{q}}_{\mathrm{tot},h}^+, \mathbf{q}_{\mathrm{tot},h}^-, \bar{\mu}_h^l, \bar{\mu}_h^+, \bar{\mu}_h^-, \bar{\lambda}_h^l, \bar{\lambda}_h^+, \bar{\lambda}_h^-\right) \in (P_D^1(\mathcal{T}_h))^n \times RT_{-1}^0(\mathcal{T}_h) \times RT_{-1}^0(\mathcal{T}_h) \times RT_{-1}^0(\mathcal{T}_h) \times M_{-1}^0(\mathcal{T}_h) \times M_{-1}^0(\mathcal{T}_h) \times M_{-1}^0(\mathcal{T}_h) \times M_{-1,D}^0(\mathcal{E}_h) \times M_{-1,D}^0(\mathcal{E}_h) \times M_{-1,D}^0(\mathcal{E}_h)$ and $t > 0$.

Note that in the above variational formulation the values for φ_h and c_h^β are calculated from the secondary equations mentioned in (2.7.7).

Let $\mathbf{x}_i$, $i = 1, \ldots, I$, be numbered nodes of the triangulation $\{\mathbf{x} \in \mathcal{T}_h : \mathbf{x} \notin \overline{\Gamma}_{\mathbf{u}}^D\}$; T_k, $k = 1, \ldots, K$, be numbered sub-domains of $\mathcal{T}_h$ and $e_j^{(T)}$, $j = 1, \ldots, J^{(T)}$, be the edges ($n = 2$) or faces ($n = 3$) of T for each $T \in \mathcal{T}_h$.

Recall that the finite-dimensional space $RT_{-1}^0(\mathcal{T}_h)$ is spanned by the linearly independent vectorial basis functions $\mathbf{v}_j^{(T)}$, $j = 1, \ldots, J^{(T)}$, $T \in \mathcal{T}_h$, such that $\mathbf{v}_j^{(T)}$

has its support in T and

$$\int_{e_{j'}^{(T)}} \mathbf{n}_t \cdot \mathbf{v}_j^{(T)}\, ds = \delta_{jj'}, \quad j, j' = 1, \ldots, J^{(T)}.$$

Thus a function $\mathbf{q} \in RT^0_{-1}(\mathcal{T}_h)$ has $J^{(T)}$ degrees of freedom per sub-domain $T \in \mathcal{T}_h$ and in total $J = \sum_{T\in\mathcal{T}_h} J^{(T)}$ degrees of freedom in $\mathcal{T}_h$. The degrees of freedom of $\mathbf{q}$ in the sub-domain $T \in \mathcal{T}_h$ are equal to

$$\int_{e_j^{(T)}} \mathbf{n}_T \cdot \mathbf{q}\, ds, \quad j = 1, \ldots J^{(T)}.$$

Recall that the finite-dimensional space $M^0_{-1}(\mathcal{T}_h)$ is spanned by the linearly independent scalar basis functions ψ_k, $k = 1, \ldots, K$, such that (4.2.42) holds.

Let e_l, $l = 1, \ldots, L$, be the numbered edges $(n = 2)$ or faces $(n = 3)$ of $\{e \in \mathcal{E}_h : e \not\subset \overline{\Gamma}_p^D\}$. The finite-dimensional space $M^0_{-1,D}(\mathcal{E}_h)$ is spanned by the linearly independent scalar basis functions η_l, $l = 1, \ldots, L$, such that

$$\eta_l(\mathbf{x}) = \delta_{ll'}, \quad \mathbf{x} \in e_{l'}, \quad l, l' = 1, \ldots, L.$$

Therefore a function $\lambda \in M^0_{-1,D}(\mathcal{E}_h)$ has one degree of freedom per edge e_l, $l = 1, \ldots, L$, which is equal to its constant value on e_l.

Now by definition, functions $\mathbf{u}_h$, μ_h^l, μ_h^β, $\mathbf{q}_h^l$, $\mathbf{q}_{\mathrm{tot},h}^\beta$, λ_h^l and λ_h^β are expressed as

$$\begin{aligned}
\mathbf{u}_h(\mathbf{x}, t) &= \sum_{i=1}^{I} \tilde{u}_i(t)\mathbf{w}_i(\mathbf{x}), \\
\mathbf{q}_h^l(\mathbf{x}, t) &= \sum_{j=1}^{J} \tilde{\mathbf{q}}_j^l(t)\mathbf{v}_j(\mathbf{x}), \\
\mathbf{q}_{\mathrm{tot},h}^\beta(\mathbf{x}, t) &= \sum_{j=1}^{J} \tilde{\mathbf{q}}_{\mathrm{tot},j}^\beta(t)\mathbf{v}_j(\mathbf{x}), \qquad \beta = +, -, \\
\mu_h^l(\mathbf{x}, t) &= \sum_{k=1}^{K} \tilde{\mu}_k^l(t)\psi_k(\mathbf{x}), \\
\mu_h^\beta(\mathbf{x}, t) &= \sum_{k=1}^{K} \tilde{\mu}_k^\beta(t)\psi_k(\mathbf{x}), \qquad \beta = +, -, \\
\lambda_h^l(\mathbf{x}, t) &= \lambda_{in}^l + \sum_{\ell=1}^{L} \tilde{\lambda}_\ell^l(t)\eta_\ell(\mathbf{x}), \\
\lambda_h^\beta(\mathbf{x}, t) &= \lambda_{in}^\beta + \sum_{\ell=1}^{L} \tilde{\lambda}_\ell^\beta(t)\eta_\ell(\mathbf{x}), \qquad \beta = +, -,
\end{aligned}$$

where λ_{in}^{β}, $\beta = l, +, -$, are defined by

$$\lambda_{in}^{\beta} \in M_{-1}^{0}(\mathcal{E}_h) \quad \text{and} \quad \begin{cases} \lambda_{in}^{\beta} = \tilde{\mu}_{in}^{\beta} & \text{on } \Gamma_p^D, \\ \lambda_{in}^{\beta} = 0 & \text{on } \bigcup\limits_{e \in \mathcal{E}_h} e \backslash \Gamma_p^D. \end{cases}$$

Substituting this in the mixed-hybrid variational formulation gives

$$\boxed{\mathfrak{A}(\varphi_h, c_h^+, c_h^-)\frac{d\mathbf{y}}{dt} + \mathfrak{B}(\varphi_h, c_h^+, c_h^-)\mathbf{y} = \mathfrak{F}(\varphi_h, c_h^+, c_h^-) + \frac{d\mathfrak{G}}{dt}(\varphi_h, c_h^+, c_h^-),} \tag{5.2.10}$$

where $\mathfrak{A}(\varphi_h, c_h^+, c_h^-)$ and $\mathfrak{B}(\varphi_h, c_h^+, c_h^-)$ are

$$\mathfrak{A}(\varphi_h, c_h^+, c_h^-)_{ij} = \begin{cases} \mathbf{B}^T, & i = 5,\ j = 1, \\ \\ \mathbf{0}, & i \neq 5,\ j \neq 1, \end{cases}$$

$$\mathfrak{B}(\varphi_h, c_h^+, c_h^-) =$$

$$\left(\begin{array}{cccccccccc} \mathbf{A} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{B} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{C}^{ll}(\varphi_h/c_h^{\beta}) & \mathbf{C}^{l+}(\varphi_h) & \mathbf{C}^{l-}(\varphi_h) & \mathbf{D} & \mathbf{0} & \mathbf{0} & \mathbf{E} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{C}^{l+}(\varphi_h) & \mathbf{C}^{++}(\varphi_h c_h^+) & \mathbf{0} & \mathbf{0} & \mathbf{D} & \mathbf{0} & \mathbf{0} & \mathbf{E} & \mathbf{0} \\ \mathbf{0} & \mathbf{C}^{l-}(\varphi_h) & \mathbf{0} & \mathbf{C}^{--}(\varphi_h c_h^-) & \mathbf{0} & \mathbf{0} & \mathbf{D} & \mathbf{0} & \mathbf{0} & \mathbf{E} \\ \mathbf{0} & \mathbf{D}^T & \mathbf{0} & \mathbf{0} & & & & & & \\ \mathbf{0} & \mathbf{0} & \mathbf{D}^T & \mathbf{0} & & & & & & \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{D}^T & & & & & & \\ \mathbf{0} & \mathbf{E}^T & \mathbf{0} & \mathbf{0} & & & \mathbf{0}_{3(K+L)\times 3(K+L)} & & & \\ \mathbf{0} & \mathbf{0} & \mathbf{E}^T & \mathbf{0} & & & & & & \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{E}^T & & & & & & \end{array}\right)$$

respectively, and

$$\begin{aligned} \mathbf{y} &= \left[\tilde{\mathbf{u}}, \tilde{\mathbf{q}}^l, \tilde{\mathbf{q}}_{\mathrm{tot}}^+, \tilde{\mathbf{q}}_{\mathrm{tot}}^-, \tilde{\boldsymbol{\mu}}^l, \tilde{\boldsymbol{\mu}}^+, \tilde{\boldsymbol{\mu}}^-, \tilde{\boldsymbol{\lambda}}^l, \tilde{\boldsymbol{\lambda}}^+, \tilde{\boldsymbol{\lambda}}^-\right]^T, \\ \mathfrak{F}(\varphi_h, c_h^+, c_h^-) &= \left[\mathbf{F}, \mathbf{F}_1^l, \mathbf{F}_1^+, \mathbf{F}_1^-, \mathbf{0}, \mathbf{0}, \mathbf{0}, \mathbf{0}, \mathbf{0}, \mathbf{0}\right]^T \\ \mathfrak{G}(\varphi_h, c_h^+, c_h^-) &= \left[\mathbf{0}, \mathbf{0}, \mathbf{0}, \mathbf{0}, \mathbf{0}, \mathbf{F}_2^+, \mathbf{F}_2^-, \mathbf{0}, \mathbf{0}, \mathbf{0}\right]^T. \end{aligned}$$

In the above formulations,

$$
\begin{aligned}
\tilde{\mathbf{u}} &= [\tilde{u}_1 \cdots, \tilde{u}_{nI}]^T, \\
\tilde{\mathbf{q}} &= [\tilde{q}_1, \cdots, \tilde{q}_J]^T, \\
\tilde{\mathbf{q}}^{\beta}_{\mathrm{tot}} &= [\tilde{q}^{\beta}_{\mathrm{tot},1}, \cdots, \tilde{q}^{\beta}_{\mathrm{tot},J}]^T, \qquad \beta = +, -, \\
\tilde{\boldsymbol{\mu}}^{l} &= [\tilde{\mu}^{l}_1, \cdots, \tilde{\mu}^{l}_K]^T, \\
\tilde{\boldsymbol{\mu}}^{\beta} &= [\tilde{\mu}^{\beta}_1, \cdots, \tilde{\mu}^{\beta}_K]^T, \qquad \beta = +, -, \\
\tilde{\boldsymbol{\lambda}}^{l} &= [\tilde{\lambda}^{l}_1, \cdots, \tilde{\lambda}^{l}_L]^T, \\
\tilde{\boldsymbol{\lambda}}^{\beta} &= [\tilde{\lambda}^{\beta}_1, \cdots, \tilde{\lambda}^{\beta}_L]^T, \qquad \beta = +, -, \\
\mathbf{A}_{ij} &= \int_{\Omega} (2\mu_s \boldsymbol{\mathcal{E}}(\mathbf{w}_i) : \boldsymbol{\mathcal{E}}(\mathbf{w}_j) + \lambda_s \nabla \cdot \mathbf{w}_i \nabla \cdot \mathbf{w}_j)\, d\mathbf{x}, \\
\mathbf{B}_{ij} &= -\int_{T_j} \nabla \cdot \mathbf{w}_i \, d\mathbf{x}, \\
\mathbf{C}^{ll}_{ij}(\varphi_h / c^{\beta}_h) &= \frac{1}{K} \int_{\Omega} \mathbf{v}_i \cdot \mathbf{v}_j \, d\mathbf{x} + \sum_{\beta=+,-} \frac{RT}{D^{\beta}} \int_{\Omega} \frac{c^{\beta}_h \mathbf{v}_i \cdot \mathbf{v}_j}{\varphi_h} \, d\mathbf{x}, \\
\mathbf{C}^{l\beta}_{ij}(\varphi_h) &= -\frac{RT}{D^{\beta}} \int_{\Omega} \frac{\mathbf{v}_i \cdot \mathbf{v}_j}{\varphi_h} \, d\mathbf{x}, \quad \beta = +, -, \\
\mathbf{C}^{\beta\beta}(\varphi_h c^{\beta}_h) &= \frac{RT}{D^{\beta}} \int_{\Omega} \frac{\mathbf{v}_i \cdot \mathbf{v}_j}{\varphi_h c^{\beta}_h} \, d\mathbf{x}, \quad \beta = +, -, \\
\mathbf{D}_{ij} &= -\int_{T_j} \nabla \cdot \mathbf{v}_i \, d\mathbf{x}, \\
\mathbf{E}_{ik} &= \int_{e_k} \mathbf{n}_i \cdot \mathbf{v}_i \, ds, \\
\mathbf{F}_i &= \int_{\Omega} \Big(RT(\Gamma^+ c^+_h + \Gamma^- c^-_h) - \mu^l_0 - p_{in} \Big) \nabla \cdot \mathbf{w}_i \, d\mathbf{x} + \int_{\Gamma^N_{\mathbf{u}}} \mathbf{g}^N_{\mathbf{u}} \cdot \mathbf{w}_i \, ds, \\
(\mathbf{F}^l_1)_i &= -\int_{\Gamma} \tilde{\mu}^l_{in} \mathbf{n} \cdot \mathbf{v}_i \, ds, \\
(\mathbf{F}^{\beta}_1)_i &= -\int_{\Gamma} \tilde{\mu}^{\beta}_{in} \mathbf{n} \cdot \mathbf{v}_i \, ds, \quad \beta = +, -, \\
(\mathbf{F}^{\beta}_2)_i(\varphi_h c^{\beta}_h) &= \int_{T_i} (\nabla \cdot \mathbf{u}_h + \varphi_0)\, c^{\beta}_h \, d\mathbf{x}, \quad \beta = +, -.
\end{aligned}
$$

Remark 5.4. *From now in our notations, we omit the dependencies of the matrix and right-hand side functions to φ_h, c^+_h, c^-_h. We keep in mind that this is just to make our formulas more readable.*

Define

$$\mathfrak{C} = \begin{pmatrix} \mathbf{C}^{ll} & \mathbf{C}^{l+} & \mathbf{C}^{l-} \\ \mathbf{C}^{l+} & \mathbf{C}^{++} & \mathbf{0} \\ \mathbf{C}^{l-} & \mathbf{0} & \mathbf{C}^{--} \end{pmatrix}, \quad \mathfrak{D} = \begin{pmatrix} \mathbf{D} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{D} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{D} \end{pmatrix}, \quad \mathfrak{E} = \begin{pmatrix} \mathbf{E} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{E} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{E} \end{pmatrix}. \tag{5.2.11}$$

Theorem 5.5. $(\mathfrak{D}|\mathfrak{E})^T\mathfrak{C}^{-1}(\mathfrak{D}|\mathfrak{E})$ *is a symmetric positive-definite matrix.*

Proof. $\mathfrak{C}$ is symmetric positive-definite and $(\mathfrak{D}|\mathfrak{E})^T\mathfrak{C}^{-1}(\mathfrak{D}|\mathfrak{E})$ is symmetric positive semi-definite. To prove the positive-definiteness, we need to show that $(\mathfrak{D}|\mathfrak{E})$ has full rank. Suppose

$$(\mathfrak{D}|\mathfrak{E})\left[\tilde{\boldsymbol{\mu}}^l, \tilde{\boldsymbol{\mu}}^+, \tilde{\boldsymbol{\mu}}^-, \tilde{\boldsymbol{\lambda}}^l, \tilde{\boldsymbol{\lambda}}^+, \tilde{\boldsymbol{\lambda}}^-\right]^T = \mathbf{0},$$

then

$$\begin{cases} \mathbf{D}\tilde{\boldsymbol{\mu}}^l + \mathbf{E}\tilde{\boldsymbol{\lambda}}^l = \mathbf{0}, \\ \mathbf{D}\tilde{\boldsymbol{\mu}}^+ + \mathbf{E}\tilde{\boldsymbol{\lambda}}^+ = \mathbf{0}, \\ \mathbf{D}\tilde{\boldsymbol{\mu}}^- + \mathbf{E}\tilde{\boldsymbol{\lambda}}^- = \mathbf{0}. \end{cases} \tag{5.2.12}$$

Since

$$\begin{aligned} & \mathbf{D}\tilde{\boldsymbol{\mu}}^l + \mathbf{E}\tilde{\boldsymbol{\lambda}}^l = 0 \Leftrightarrow \mathbf{v}^T(\mathbf{D}\tilde{\boldsymbol{\mu}}^l + \mathbf{E}\tilde{\boldsymbol{\lambda}}^l) = 0 \quad \text{for all } \mathbf{v} \in \mathbb{R}^J \\ \Leftrightarrow \quad & \sum_{T\in\mathcal{T}_h}\left(\int_T \mu_h^l \nabla\cdot\mathbf{v}_h\, d\mathbf{x} - \int_{\partial T}\lambda_h^l \mathbf{n}_T\cdot\mathbf{v}_h\, ds\right) = 0 \quad \text{for all } \mathbf{v}_h \in RT_{-1}^0(\mathcal{T}_h) \\ \Leftrightarrow \quad & \sum_{T\in\mathcal{T}_h}\int_{\partial T}(\mu_h^l - \lambda_h^l)\mathbf{n}_T\cdot\mathbf{v}_h\, ds = 0 \quad \text{for all } \mathbf{v}_h \in RT_{-1}^0(\mathcal{T}_h) \\ \Leftrightarrow \quad & \mu_h^l = \lambda_h^l \text{ on } \partial T \quad \text{for all } T \in \mathcal{T}_h \Leftrightarrow \mu_h^l = 0 \text{ in } \Omega, \quad \lambda_h^l = 0 \text{ on } \bigcup_{e\in\mathcal{E}_h} e \\ \Leftrightarrow \quad & \tilde{\boldsymbol{\mu}}^l = 0, \quad \tilde{\boldsymbol{\lambda}}^l = 0, \end{aligned}$$

where

$$\begin{aligned} \mu_h^l(\mathbf{x},t) &= \sum_{k=1}^K \tilde{\mu}_k^l(t)\psi_k(\mathbf{x}) \in M_{-1}^0(\mathcal{T}_h), \\ \lambda_h^l(\mathbf{x},t) &= \sum_{\ell=1}^L \tilde{\lambda}_\ell^l(t)\eta_\ell(\mathbf{x}) \in M_{-1}^0(\mathcal{E}_h). \end{aligned}$$

Therefore we have

$$(\mathfrak{D}\boldsymbol{\Lambda}_1 + \mathfrak{E}\boldsymbol{\Lambda}_2)^T\,\mathfrak{C}^{-1}\,(\mathfrak{D}\boldsymbol{\Lambda}_1 + \mathfrak{E}\boldsymbol{\Lambda}_2) > 0 \tag{5.2.13}$$

for all $(\boldsymbol{\Lambda}_1, \boldsymbol{\Lambda}_2) \in \mathbb{R}^{3(K+L)}\backslash\{\mathbf{0}\}$. ■

In the sequel the hybridization technique will be proceeded. Note that the system (5.2.10) can be considered as

$$\begin{cases} \mathbf{A}\tilde{\mathbf{u}} + \mathbf{B}\tilde{\boldsymbol{\mu}}^l = \mathbf{F}, \\ \mathfrak{C}\begin{pmatrix} \tilde{\mathbf{q}}^l \\ \tilde{\mathbf{q}}^+_{\mathrm{tot}} \\ \tilde{\mathbf{q}}^-_{\mathrm{tot}} \end{pmatrix} + (\mathfrak{D}|\mathfrak{E})\begin{pmatrix} \tilde{\boldsymbol{\mu}}^l \\ \tilde{\boldsymbol{\mu}}^+ \\ \tilde{\boldsymbol{\mu}}^- \\ \tilde{\boldsymbol{\lambda}}^l \\ \tilde{\boldsymbol{\lambda}}^+ \\ \tilde{\boldsymbol{\lambda}}^- \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{pmatrix}, \\ \begin{pmatrix} \mathbf{B}^T \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{pmatrix} \frac{d}{dt}\tilde{\mathbf{u}} + (\mathfrak{D}|\mathfrak{E})^T \begin{pmatrix} \tilde{\mathbf{q}}^l \\ \tilde{\mathbf{q}}^+_{\mathrm{tot}} \\ \tilde{\mathbf{q}}^-_{\mathrm{tot}} \end{pmatrix} = \frac{d}{dt}\begin{pmatrix} \mathbf{0} \\ \mathbf{F}_2^+ \\ \mathbf{F}_2^- \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{pmatrix} \end{cases} \tag{5.2.14}$$

In the system (5.2.14) $\mathfrak{C}$ is symmetric positive definite matrix and can be inverted at the finite element level. Therefore the second equation in (5.2.14) implies

$$\boxed{\begin{pmatrix} \tilde{\mathbf{q}}^l \\ \tilde{\mathbf{q}}^+_{\mathrm{tot}} \\ \tilde{\mathbf{q}}^-_{\mathrm{tot}} \end{pmatrix} = -\mathfrak{C}^{-1}(\mathfrak{D}|\mathfrak{E})\begin{pmatrix} \tilde{\boldsymbol{\mu}}^l \\ \tilde{\boldsymbol{\mu}}^+ \\ \tilde{\boldsymbol{\mu}}^- \\ \tilde{\boldsymbol{\lambda}}^l \\ \tilde{\boldsymbol{\lambda}}^+ \\ \tilde{\boldsymbol{\lambda}}^- \end{pmatrix}}. \tag{5.2.15}$$

Using (5.2.15) and the third equation in (5.2.14) we get

$$\begin{pmatrix} \mathbf{B}^T \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{pmatrix} \frac{d}{dt}\tilde{\mathbf{u}} - (\mathfrak{D}|\mathfrak{E})^T\mathfrak{C}^{-1}(\mathfrak{D}|\mathfrak{E})\begin{pmatrix} \tilde{\boldsymbol{\mu}}^l \\ \tilde{\boldsymbol{\mu}}^+ \\ \tilde{\boldsymbol{\mu}}^- \\ \tilde{\boldsymbol{\lambda}}^l \\ \tilde{\boldsymbol{\lambda}}^+ \\ \tilde{\boldsymbol{\lambda}}^- \end{pmatrix} = \frac{d}{dt}\begin{pmatrix} \mathbf{0} \\ \mathbf{F}_2^+ \\ \mathbf{F}_2^- \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{pmatrix}. \tag{5.2.16}$$

In the next step we solve the above equation for $[\tilde{\boldsymbol{\mu}}^l, \tilde{\boldsymbol{\mu}}^+, \tilde{\boldsymbol{\mu}}^-]^T$. To do this, we need to state the following lemma.

Lemma 5.6. *$\mathfrak{D}^T\mathfrak{C}^{-1}\mathfrak{D}$ is a symmetric positive definite matrix.*

Proof. Since $\mathfrak{C}$ is symmetric positive definite, $\mathfrak{D}^T\mathfrak{C}^{-1}\mathfrak{D}$ is symmetric positive semi-definite. In order to prove that this matrix is positive definite, we need to find the null space of it.
Let $\mathfrak{D}\tilde{\mu}^\beta = 0$, $\beta = l, +, -$, then

$$\sum_{T\in\mathcal{T}_h}\int_T \mu_h^\beta \nabla\cdot\mathbf{v}_h\, d\mathbf{x} = 0 \text{ for all } \mathbf{v}_h \in RT^0_{-1}(\mathcal{T}_h), \quad \beta = l, +, -, .$$

$\mathbf{v}_h$ is assumed to be continuous inside each element T, therefore the above summation will reduce to each element T. With an appropriate choice of $\mathbf{v}_h$, we can take $\nabla\cdot\mathbf{v}_h$ to be equal to 1 in T, therefore we have

$$\int_T \mu_h^\beta\, d\mathbf{x} = 0 \quad \text{for all } T\in\mathcal{T}_h, \quad \beta = l, +, -.$$

Hence

$$\mu_h^\beta\Big|_T = 0 \quad \text{for all } T\in\mathcal{T}_h, \quad \beta = l, +, -.$$

This results in the symmetric positive definiteness of $\mathfrak{D}^T\mathfrak{C}^{-1}\mathfrak{D}$. ■

Remark 5.7. *It can be seen that $\mathfrak{D}^T\mathfrak{C}^{-1}\mathfrak{D}$ is similar to a block diagonal matrix. In fact, we need to define an appropriate permutation matrix. Define $\mathbf{P}$ after reordering the rows of an identity matrix $\mathbf{I}_{3L\times 3L}$ based on the vector $(1, L+1, 2L+1, 2, L+2, 2L+2, \cdots, L, 2L, 3L)$. Then it can be seen that the matrix $\mathbf{P}(\mathfrak{D}^T\mathfrak{C}^{-1}\mathfrak{D})\mathbf{P}^{-1}$ is a block diagonal matrix and has K blocks which are 3×3 matrices and the inverse is block diagonal too. This will imply that the inverse of $\mathfrak{D}^T\mathfrak{C}^{-1}\mathfrak{D}$ has the same pattern as $\mathfrak{D}^T\mathfrak{C}^{-1}\mathfrak{D}$.*

Now by applying the above lemma and using equation (5.2.16), $[\tilde{\boldsymbol{\mu}}^l, \tilde{\boldsymbol{\mu}}^+, \tilde{\boldsymbol{\mu}}^-]^T$ can be expressed as

$$\boxed{\begin{aligned}\begin{pmatrix}\tilde{\boldsymbol{\mu}}^l\\ \tilde{\boldsymbol{\mu}}^+\\ \tilde{\boldsymbol{\mu}}^-\end{pmatrix} &= (\mathfrak{D}^T\mathfrak{C}^{-1}\mathfrak{D})^{-1}\left[-\mathfrak{D}^T\mathfrak{C}^{-1}\mathfrak{E}\begin{pmatrix}\tilde{\boldsymbol{\lambda}}^l\\ \tilde{\boldsymbol{\lambda}}^+\\ \tilde{\boldsymbol{\lambda}}^-\end{pmatrix}\right.\\ &+ \left.\begin{pmatrix}\mathbf{B}^T\\ \mathbf{0}\\ \mathbf{0}\end{pmatrix}\frac{d}{dt}\tilde{\mathbf{u}} - \frac{d}{dt}\begin{pmatrix}\mathbf{0}\\ \mathbf{F}_2^+\\ \mathbf{F}_2^-\end{pmatrix}\right].\end{aligned}} \tag{5.2.17}$$

If we substitute (5.2.17) in the system (5.2.14), then this system reduces to

$$\boxed{\begin{pmatrix}\mathbf{A}\tilde{\mathbf{u}}\\ \mathbf{0}\end{pmatrix} + \begin{pmatrix}\mathfrak{A}_1 & \mathfrak{A}_2\\ \mathfrak{A}_2^T & -\mathfrak{A}_3\end{pmatrix}\begin{pmatrix}\frac{d}{dt}\tilde{\mathbf{u}}\\ \tilde{\boldsymbol{\lambda}}^l\\ \tilde{\boldsymbol{\lambda}}^+\\ \tilde{\boldsymbol{\lambda}}^-\end{pmatrix} = \begin{pmatrix}\mathbf{F}_1\\ \mathbf{0}\end{pmatrix} + \begin{pmatrix}\mathfrak{F}_1\\ \mathfrak{F}_2\end{pmatrix}\frac{d}{dt}\begin{pmatrix}\mathbf{0}\\ \mathbf{F}_2^+\\ \mathbf{F}_2^-\end{pmatrix},}$$

(5.2.18)

where $\mathfrak{A}_1, \mathfrak{A}_1$ and $\mathfrak{A}_3$ are

$$\mathfrak{A}_1 = \begin{pmatrix} \mathbf{B} & \mathbf{0} & \mathbf{0} \end{pmatrix} (\mathfrak{D}^T \mathfrak{C}^{-1} \mathfrak{D})^{-1} \begin{pmatrix} \mathbf{B}^T \\ \mathbf{0} \\ \mathbf{0} \end{pmatrix}, \tag{5.2.19}$$

$$\mathfrak{A}_2 = -\begin{pmatrix} \mathbf{B} & \mathbf{0} & \mathbf{0} \end{pmatrix} (\mathfrak{D}^T \mathfrak{C}^{-1} \mathfrak{D})^{-1} (\mathfrak{D}^T \mathfrak{C}^{-1} \mathfrak{E}), \tag{5.2.20}$$

$$\mathfrak{A}_3 = -(\mathfrak{E}^T \mathfrak{C}^{-1} \mathfrak{D})(\mathfrak{D}^T \mathfrak{C}^{-1} \mathfrak{D})^{-1} (\mathfrak{D}^T \mathfrak{C}^{-1} \mathfrak{E}) + (\mathfrak{E}^T \mathfrak{C}^{-1} \mathfrak{E}). \tag{5.2.21}$$

$\mathfrak{F}_1$ and $\mathfrak{F}_2$ can be derived as

$$\mathfrak{F}_1 = \begin{pmatrix} \mathbf{B} & \mathbf{0} & \mathbf{0} \end{pmatrix} (\mathfrak{D}^T \mathfrak{C}^{-1} \mathfrak{D})^{-1}, \tag{5.2.22}$$

$$\mathfrak{F}_2 = -(\mathfrak{E}^T \mathfrak{C}^{-1} \mathfrak{D})(\mathfrak{D}^T \mathfrak{C}^{-1} \mathfrak{D})^{-1}. \tag{5.2.23}$$

Remark 5.8. *From Theorem 5.5 it follows that*

$$\boldsymbol{\eta}^T \mathfrak{A}_3 \boldsymbol{\eta} = (\mathfrak{D}\boldsymbol{\eta}_1 + \mathfrak{E}\boldsymbol{\eta}_2)^T \, \mathfrak{C}^{-1} \, (\mathfrak{D}\boldsymbol{\eta}_1 + \mathfrak{E}\boldsymbol{\eta}_2) > 0 \;\; \textit{for all} \;\; \boldsymbol{\eta}_2 \in \mathbb{R}^{3K} \backslash \{0\}, \tag{5.2.24}$$

where

$$\boldsymbol{\eta}_1 = -(\mathfrak{D}\mathfrak{C}^{-1}\mathfrak{D})^{-1} \mathfrak{D}^T \mathfrak{C}^{-1} \mathfrak{E} \boldsymbol{\eta}_2, \quad \boldsymbol{\eta} = (\boldsymbol{\eta}_1, \boldsymbol{\eta}_2).$$

Therefore $\mathfrak{A}_3$ is a symmetric positive definite matrix.

Remark 5.9. *By using the above remark, we can take one more step to solve the system for*

$$\begin{pmatrix} \tilde{\boldsymbol{\lambda}}^l \\ \tilde{\boldsymbol{\lambda}}^+ \\ \tilde{\boldsymbol{\lambda}}^- \end{pmatrix} = \mathfrak{A}_3^{-1} \left[\mathfrak{A}_2^T \frac{d}{dt} \tilde{\mathbf{u}} - \mathfrak{F}_2 \frac{d}{dt} \begin{pmatrix} \mathbf{0} \\ \mathbf{F}_2^+ \\ \mathbf{F}_2^- \end{pmatrix} \right], \tag{5.2.25}$$

whence system (5.2.18) *is reduced to*

$$\boxed{\left(\mathfrak{A}_1 + \mathfrak{A}_2 \mathfrak{A}_3^{-1} \mathfrak{A}_2^T\right) \frac{d}{dt} \tilde{\mathbf{u}} + \mathbf{A} \tilde{\mathbf{u}} = \left(\mathfrak{F}_1 + \mathfrak{A}_2 \mathfrak{A}_3^{-1} \mathfrak{F}_2\right) \frac{d}{dt} \begin{pmatrix} \mathbf{0} \\ \mathbf{F}_2^+ \\ \mathbf{F}_2^- \end{pmatrix}.} \tag{5.2.26}$$

Remark 5.10. *Note that in computation of $\mathfrak{A}_1$, $\mathfrak{A}_2$ and $\mathfrak{A}_3$, the inverse of the matrix $\mathfrak{D}\mathfrak{C}^{-1}\mathfrak{D}$ is needed. In Remark 5.9 we have seen that this inverse can be calculated per finite element. This is an important fact in using the hybridization technique.*

Let Δt be the time step and $\left(\tilde{\mathbf{u}}^n, \tilde{\boldsymbol{\lambda}}^{l,n}, \tilde{\boldsymbol{\lambda}}^{+,n}, \tilde{\boldsymbol{\lambda}}^{-,n}\right)$ the approximation of the solution vector $\left(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\lambda}}^l, \tilde{\boldsymbol{\lambda}}^+, \tilde{\boldsymbol{\lambda}}^-\right)$ at $t = t_n = n\Delta t$. Then the nonlinear system of equation

(5.2.18) resulting from backward Euler is:

$$\begin{pmatrix} \mathbf{A}\tilde{\mathbf{u}}^{n+1} \\ \mathbf{0} \end{pmatrix} + \begin{pmatrix} \mathfrak{A}_1\left(\varphi_h^{n+1}, c_h^{+,n+1}, c_h^{-,n+1}\right) & \mathfrak{A}_2\left(\varphi_h^{n+1}, c_h^{+,n+1}, c_h^{-,n+1}\right) \\ \mathfrak{A}_2^T\left(\varphi_h^{n+1}, c_h^{+,n+1}, c_h^{-,n+1}\right) & -\mathfrak{A}_3\left(\varphi_h^{n+1}, c_h^{+,n+1}, c_h^{-,n+1}\right) \end{pmatrix}$$
$$\times \begin{pmatrix} \dfrac{\tilde{\mathbf{u}}^{n+1} - \tilde{\mathbf{u}}^n}{\Delta t} \\ \tilde{\boldsymbol{\lambda}}^{l,n+1} \\ \tilde{\boldsymbol{\lambda}}^{+,n+1} \\ \tilde{\boldsymbol{\lambda}}^{-,n+1} \end{pmatrix} = \begin{pmatrix} \mathbf{F}_1 \\ \mathbf{0} \end{pmatrix} + \begin{pmatrix} \mathfrak{F}_1\left(\varphi_h^{n+1}, c_h^{+,n+1}, c_h^{-,n+1}\right) \\ \mathfrak{F}_2\left(\varphi_h^{n+1}, c_h^{+,n+1}, c_h^{-,n+1}\right) \end{pmatrix}$$
$$\times \begin{pmatrix} \mathbf{0} \\ \dfrac{\mathbf{F}_2^+\left(\varphi_h^{n+1}, c_h^{+,n+1}, c_h^{-,n+1}\right) - \mathbf{F}_2^+\left(\varphi_h^n, c_h^{+,n}, c_h^{-,n}\right)}{\Delta t} \\ \dfrac{\mathbf{F}_2^-\left(\varphi_h^{n+1}, c_h^{+,n+1}, c_h^{-,n+1}\right) - \mathbf{F}_2^-\left(\varphi_h^n, c_h^{+,n}, c_h^{-,n}\right)}{\Delta t} \end{pmatrix}. \tag{5.2.27}$$

The assumption that c_h^β, $\beta = +, -$, and φ_h are known transforms the system into a linear one. For φ_h the value at the old time step is taken. Thus the value of c_h^{fc} at the old time level is known and therefore the difference $c_h^+ - c_h^-$ by electro-neutrality. Define $c^\pm = c^+ + c^-$, then the solution $\tilde{\boldsymbol{\mu}}_h^\beta$ from (5.2.17) and (5.2.27) for fixed c_h^β, $\beta = +, -$, can be denoted symbolically by $(\tilde{\boldsymbol{\mu}}_h^+, \tilde{\boldsymbol{\mu}}_h^-) = \mathsf{A}^{-1}(c_h^\pm)\mathsf{b}(c_h^\pm)$, where A and b represent the matrix and right-hand side of the linear system. Now $c_h^\pm$ can be computed by the third relation in the secondary equations in (2.7.7), i.e., $c_h^\pm = \mathsf{f}(\tilde{\boldsymbol{\mu}}_h^+, \tilde{\boldsymbol{\mu}}_h^-, c_h^\pm)$. Ergo, we obtain the non-linear system

$$c_h^\pm = \mathsf{f}\left(\mathsf{A}^{-1}(c_h^\pm)\mathsf{b}(c_h^\pm), c_h^\pm\right). \tag{5.2.28}$$

This system can be solved by an iterative procedure for non-linear system (see Algorithm 1).

In each iteration a linear system has to be solved. It should be observed that different scales are apparent in (5.2.18) 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

$$\mathsf{D}^2 = \operatorname{diag}\left(\frac{L}{\Delta t(2\mu_s + \lambda_s)}, \frac{L}{K}, \frac{RTL}{D^+\varphi_0 c_0^{fc}}, \frac{RTL}{D^-\varphi_0 c_0^{fc}}\right). \tag{5.2.29}$$

Here L is a representative length scale.

5.3 Numerical simulations

In this section the element contributions to the matrices and right-hand sides in (5.2.18) are computed.

Algorithm 1 Solving the nonlinear system (5.2.27) by using iterations

Given φ_h^n, $c_h^{\pm,n}$ and given ϵ
criteria $\Leftarrow 1$
while criteria $> \epsilon$ **do**
$c_h^{fc,n} \Leftarrow c_0^{fc} \exp\left(-\dfrac{\varphi_h^n - \varphi_0}{\varphi_0(1-\varphi_0)}\right)$
$d_h^{\pm,n} \Leftarrow c_h^{+,n} - c_h^{-,n}$ $\{= c_h^{fc,n}$ by electroneutrality$\}$
$c_h^{+,n} \Leftarrow (c_h^{\pm,n} + d_h^{\pm,n})/2$
$c_h^{-,n} \Leftarrow c_h^{\pm,n} - c_h^{+,n}$
$\left(\tilde{\mathbf{u}}^{n+1}, \tilde{\boldsymbol{\lambda}}^{l,n+1}, \tilde{\boldsymbol{\lambda}}^{+,n+1}, \tilde{\boldsymbol{\lambda}}^{-,n+1}\right) \Leftarrow$ solve the *linear* system (5.2.27)
$\left(\tilde{\boldsymbol{\mu}}^{l,n+1}, \tilde{\boldsymbol{\mu}}^{+,n+1}, \tilde{\boldsymbol{\mu}}^{-,n+1}\right) \Leftarrow$ use equation (5.2.17)
$(\tilde{\varphi}_h^{n+1}, \tilde{c}_h^{+,n+1}, \tilde{c}_h^{-,n+1}) \Leftarrow$ use the secondary equations in (2.7.7)
criteria $\Leftarrow \min_{\beta=+,-} \|\tilde{c}_h^{\beta,n+1} - c_h^{\beta,n}\|_0$
$c_h^{\beta,n} \Leftarrow \tilde{c}_h^{\beta,n+1}$, $\beta = +, -$
$\varphi_h^n \Leftarrow \tilde{\varphi}_h^{n+1}$
end while
$c_h^{\beta,n+1} \Leftarrow \tilde{c}_h^{\beta,n+1}$
$\varphi_h^{n+1} \Leftarrow \tilde{\varphi}_h^{n+1}$

The element contribution to the elasticity matrix $\mathbf{A}$ and $\mathbf{B}$ in (5.2.18) can be computed in an standard way. For element contribution to the matrices $\mathbf{C}^{\beta\gamma}$, $\beta, \gamma = l, +, -$, recall (4.4.4)

$$\left(\mathbf{C}^{(T)}_{J^{(T)}\times J^{(T)}}\right)_{ij} = \sum_{k=1}^{n} \hat{c}_{kk}^{(T)} \left(\mathbf{A}_{kk}\right)_{ij} + \sum_{k=1}^{n}\sum_{l=1}^{n-1} \hat{c}_{kl}^{(T)} \left(\mathbf{A}_{kl} + \mathbf{A}_{lk}\right)_{ij},$$

where all matrices in the summations are symmetric are given in (Kaasschieter and Huijben, 1992).

As an example we take T to be a parallelogram, where $n = 2$ and $J^{(T)} = 4$, thus we have

$$A_{11} = \frac{1}{6}\begin{pmatrix} 2 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \qquad A_{12} + A_{21} = \frac{1}{4}\begin{pmatrix} 0 & 1 & 0 & -1 \\ 1 & 0 & -1 & 0 \\ 0 & -1 & 0 & 1 \\ -1 & 0 & 1 & 0 \end{pmatrix},$$

$$A_{22} = \frac{1}{6}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 2 \end{pmatrix}.$$

Another example is a triangle where $n = 2$ and $J^{(T)} = 3$,

$$A_{11} = \frac{1}{12}\begin{pmatrix} 1 & -1 & 1 \\ -1 & 3 & -1 \\ 1 & -1 & 1 \end{pmatrix}, \qquad A_{12} + A_{21} = \frac{1}{12}\begin{pmatrix} 1 & -1 & -1 \\ -1 & -3 & 3 \\ -1 & 3 & -3 \end{pmatrix},$$

$$A_{22} = \frac{1}{12}\begin{pmatrix} 1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 3 \end{pmatrix}.$$

Using Green's formula, (4.2.30) and (4.2.35), simple formulas can be derived for the element contributions of the remaining matrices and right hand sides in (5.2.18), namely

$$\left(D^{(T)}_{J^{(T)}\times 1}\right)_i = -\int_T \nabla \cdot \mathbf{v}_i^{(T)}\, d\mathbf{x} = -1, \tag{5.3.1}$$

$$\left(G^{(T)}_{J^{(T)}\times J^{(T)}}\right)_{ik} = \int_{e_k^{(T)}} \mathbf{n}_T \cdot \mathbf{v}_i^{(T)}\, ds = \delta_{ik}, \tag{5.3.2}$$

$$F_1^{\beta} = \begin{cases} -\tilde{\mu}_{in}, & \text{if } e_i \subset \overline{\Gamma_p^D} \\ 0 & \text{otherwise.} \end{cases}, \beta = l, +, -. \tag{5.3.3}$$

The computation of $(\mathfrak{D}^T\mathfrak{C}^{-1}\mathfrak{D})^{-1}$ is essential when determining the matrices $\mathfrak{A}_i$, $(i = 1, 2, 3)$ in (5.2.19) - (5.2.21). This matrix is a block diagonal matrix (Remark 5.9) and it can thus be computed at the finite element level. The matrices $\mathfrak{A}_i$ are obtained by assembling their element contributions. The right-hand side vectors $\mathfrak{F}_1$ and $\mathfrak{F}_2$ can be computed in an analogous way.

5.3.1 Confined consolidation and free swelling

In this section, numerical solutions are calculated for confined consolidation and free swelling. To verify the method, solutions are compared with the analytical solutions from chapter 3.

The homogeneous sample is placed frictionless in a holder. Figure 5.1 illustrates the experimental setup. At the bottom $y = 0$, the sample is in contact with a glass filter saturated by a sodium chloride solution. An impermeable piston is placed on the top of the sample, $y = L$, where an external mechanical load is applied. The sample was made out of a hydrogel. A bathing solution flowed through a porous glass filter at the bottom of the sample.

Consolidation

In the consolidation experiment, we apply a load on the piston to be equal to $f(t) = -f_0\mathcal{H}(t - t_0)$, with $\mathcal{H}(t - t_0)$ the Heaviside function and $f_0 > 0$. The external concentration is kept constant during the test.

For the reference values for the electro-chemical potentials we choose

$$\mu_0^l = 2RTc_{out}, \quad \mu_0^{\beta} = -RT\ln\frac{c_{out}}{c}. \tag{5.3.4}$$

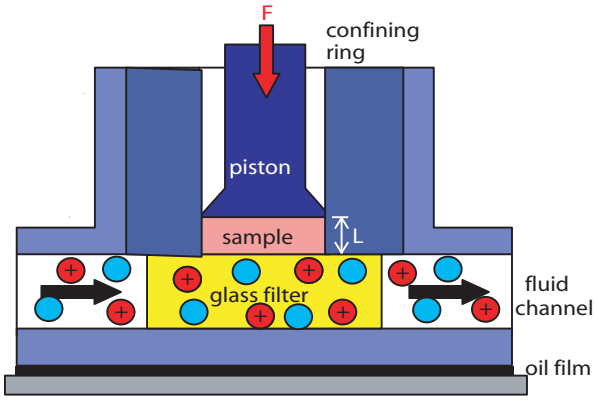


Figure 5.1. Schematic representation of the experimental set-up

By Donnan equilibrium, we know that the electro-chemical potentials are continuous at the boundary, i.e., $\mu^{\beta}_{in} = \mu^{\beta}_{out}$, $\beta = l, +, -$, where subscripts 'in' and 'out' stand for inner and outer solution, respectively.
Assume

$$\Gamma^{+}_{in} = \Gamma^{-}_{in} = \Gamma, \quad \Gamma^{+}_{out} = \Gamma^{-}_{out} = 1, \quad p_{out} = 0, \quad \xi_{out} = 0,$$

then

$$\begin{aligned} \mu^{l}_{in} &= \mu^{l}_{out} \\ &= \mu^{l}_{0} + p_{out} - 2RT\Gamma_{out}c_{out} = 0, \\ \mu^{\beta}_{in} &= \mu^{\beta}_{out} \\ &= \mu^{\beta}_{out} + z^{\beta}F\xi_{out} + RT\Gamma_{out}\ln\frac{c_{out}}{c} = 0, \quad \beta = +, -. \end{aligned}$$

Therefore, the initial and boundary conditions for the displacement and electro-chemical potentials with respect to the steady reference state $t = t_0$ are:

$$\begin{aligned} \left[\ \mu^{l} \quad \mu^{+} \quad \mu^{-}\ \right](0,t) &= \left[\ 0 \quad 0 \quad 0\ \right], \\ \left[\ \mu^{l} \quad \mu^{+} \quad \mu^{-}\ \right](y,t_0) &= \left[\ \mu^{l}_{t_0} \quad \mu^{+}_{t_0} \quad \mu^{-}_{t_0}\ \right], \\ u(0,t) &= 0, \\ u(y,t_0) &= 0, \end{aligned} \tag{5.3.5}$$

where $\left[\ \mu^{l}_{t_0} \quad \mu^{+}_{t_0} \quad \mu^{-}_{t_0}\ \right] = \left[\ f_0 \quad 0 \quad 0\ \right]$.

Free Swelling

In free swelling experiment, initially the tissue sample is at equilibrium with the external bathing solution with concentration $c_{out}(t_0^{-})$. At $t = t_0^{+}$, the concentration

of the external solution at the bottom of sample decreases to $c_{out}(t_0^+)$ instantaneously. This lowering of the concentration causes the tissue to swell to a new equilibrium state.
For the reference values of electro-chemical potentials we choose

$$\mu_0^l = 2RTc_{out}, \quad \mu_0^\beta = -RT\ln\frac{c_{out}}{c}. \tag{5.3.6}$$

The initial and boundary conditions for the displacement and electro-chemical potentials with respect to the steady reference state $t = t_0$ are:

$$\begin{aligned}
\left[\begin{array}{cccc} \mu^l & \mu^+ & \mu^- \end{array}\right](0,t) &= \left[\begin{array}{cccc} \mu^l_{in} & \mu^+_{in} & \mu^-_{in} \end{array}\right], \\
\left[\begin{array}{cccc} \mu^l & \mu^+ & \mu^- \end{array}\right](y,t_0) &= \left[\begin{array}{cccc} \mu^l_{t_0} & \mu^+_{t_0} & \mu^-_{t_0} \end{array}\right], \\
u(0,t) &= 0, \\
u(y,t_0) &= 0,
\end{aligned} \tag{5.3.7}$$

in which $\mu_{t_0}^\beta = 0$, $\beta = l, +, -$, and

$$\begin{cases}
\mu^l_{in} = & -2RT\Delta c_{out}, \\
\mu^+_{in} = & RT\ln\dfrac{c_{out}(t_0^+)}{c_{out}(t_0^-)}, \\
\mu^-_{in} = & RT\ln\dfrac{c_{out}(t_0^+)}{c_{out}(t_0^-)},
\end{cases} \tag{5.3.8}$$

$\Delta c_{out} = c_{out}(t_0^+) - c_{out}(t_0^-)$ where t_0^+ and t_0^- are the time just after and before t_0 when chemical loading is applied.

Results

In this section, the results for the confined consolidation and the free swelling are prescribed. For both computations, the parameters in the table are taken. These two experiments are taken from (Frijns, 2001) and our aim is to validate the numerical solutions by analytical solutions described in chapter 3.

Parameter	Unit	Value
$2\mu_s + \lambda_s$	MPa	4×10^3
K	$\mathrm{m^4\ N^{-1}\ s^{-1}}$	1.0×10^{-18}
c^{fc}	$\mathrm{mol\ m^{-3}}$	-2×10^2
c_{out}	$\mathrm{mol\ m^{-3}}$	1×10^2
φ		0.1
D^+	$\mathrm{m^2\ s^{-1}}$	13.3×10^{-10}
D^-	$\mathrm{m^2\ s^{-1}}$	20.3×10^{-10}
R	$\mathrm{J\ mol^{-1}\ K^{-1}}$	8.3145
T	K	293
F	$\mathrm{C\ mol^{-1}}$	96484.6
Γ		0.9

As mentioned in the previous section, an uniaxial confined swelling and compression experiment is performed on a cylindrical sample of cartilage substitute. This sample, with the diameter of 4 mm and the height of approximately 1 mm is put in an insulating conforming ring. A piston on the top of the sample is loaded mechanically. A bathing solution flows 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 of ion concentrations and electro-chemical potentials as well as pressure and voltage.

During the experiment, the mechanical and chemical load are varied. Inspired by this, two numerical simulations are considered.

Note that the problems of confined consolidation and free swelling are one dimensional with variation in the y direction only. Considering the extension of our model to higher dimensions, we would prefer to implement these one-dimensional models in a horizontally-fixed displacement two-dimensional geometry. We use a rectangle in which only vertical displacement (direction of force) is allowed with 32 vertical elements and one horizontal element. Successively, 30 increments of 20 seconds, 10 of 50 seconds and 7 of 100 seconds are used for time discretisation.

Analytical solutions for displacement, fluid pressure, electro-chemical potentials and flows for both of problems have been derived in chapter 3. Representative results from mixed hybrid finite element are compared to these solutions.

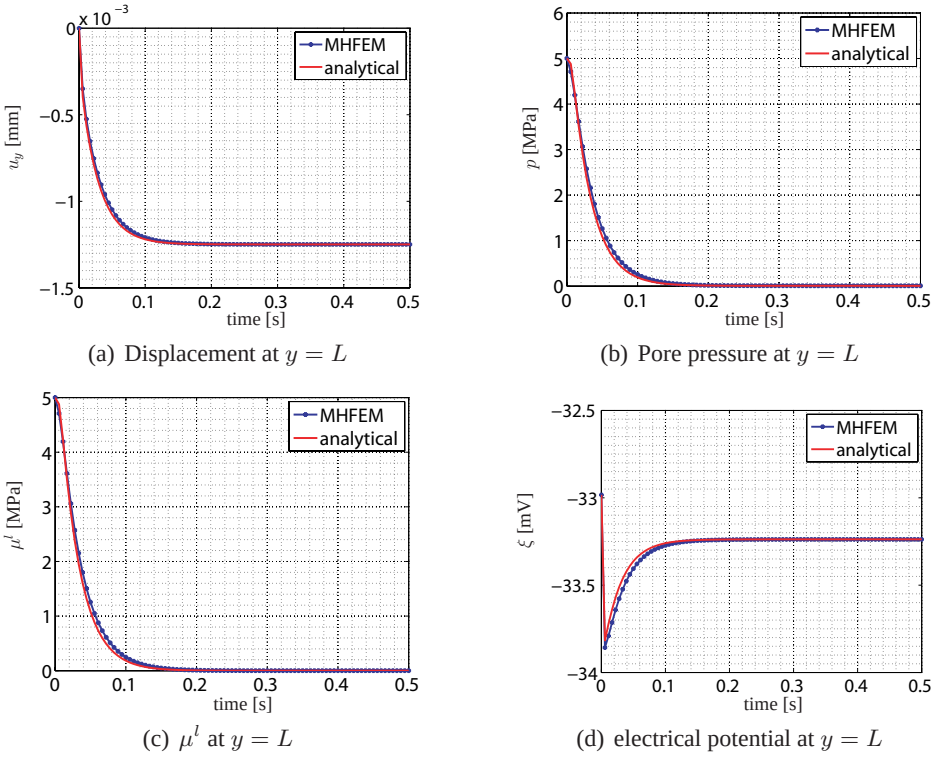
For the consolidation experiment, an inward force $f_0 = 5$ MPa is applied to the top no-flow boundary, and at the bottom rigid boundary, the porous medium is in contact with an electro-neutral bathing solution. All boundary conditions are described in (5.3.5).

The implicit Euler backward scheme is used for the time discretisation. The nonlinear system (5.2.26) is solved based on iterations for $c^{\pm}$. The criteria for convergence of this iteration is 10^{-12}. The average iterations for this problem is 10 iteration per time step and it is reduced from 15 iterations in the beginning to one when sample reaches equilibrium. We use a direct solver for the linear system. In fact, a direct solver for our one-dimensional problem is a good choice but we are aware of the fact that for higher-dimensional problems an iterative solver should be considered. Note that in this experiment, all the unknowns change immediately at $t = t_0$ s, thus another equilibrium will be establish at infinite time. At the final equilibrium, the electro-chemical potentials μ^{β}, $\beta = l, +, -$, have the same value as the values in the initial state. However, the stress and fluid pressure have changed, since the porous medium is compressed, Figures 5.2 and 5.3 display the comparison between the analytical solution and mixed hybrid finite element solutions for confined consolidation.

For the free swelling experiment, the initial and boundary conditions are chosen from (5.3.7). In this experiment, we decrease the external salt concentration with a small amount from $c_{out} = 1 \times 10^2$ mol m^{-3} to $c_{out} = 0.995 \times 10^2$ mol m^{-3}. The displacement, pore pressure, electrical potential, electro-chemical potentials and ion concentrations are displayed in Figures 5.4 and 5.5. The pore pressure increases from the initial value to the maximum value 0.0041 MPa at 0.1648 h.

The results obtained, despite the relative coarseness of the meshes are quite good. As it was expected from the mixed method, the fluid flow and ion inflows and outflows are equal per element and per time step. All functions were written in MATLAB and were run on a pentium IV (2.66 GHz).

In order to understand the nature of the mixed hybrid method, CPU checks were placed in the program at several points. First CPU time that is required to create and assemble the element matrices ($t_{elem,assem}$) is measured; then the time to solve the matrix system of equations (t_{solve}); write primary variables and compute secondary



(a) Displacement at $y = L$ (b) Pore pressure at $y = L$

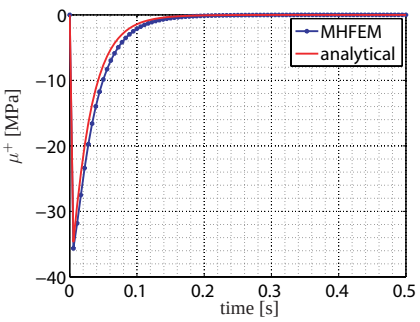
(c) μ^l at $y = L$ (d) electrical potential at $y = L$

Figure 5.2. Analytical-MHFEM comparison of the solutions for the confined consolidation (I).

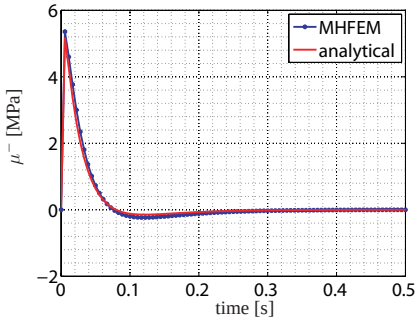
variables like φ, $c^{\pm}$ (t_{write}); time for iterations to converge ($t_{nonlinear}$).

Due to the nature of the hybridization method, the element matrix computation time and the inverse of the block diagonal matrix to get the global matrix is markedly smaller than the same procedure in the finite element code. Another reason for the hybrid method's better performance is the relatively shorter time required to compute the right-hand side at each iteration and each time step. This is due to the fact that $(\mathfrak{D}^T\mathfrak{C}^{-1}\mathfrak{D})^{-1}$ in (5.2.22) and (5.2.23) is computed per element in forming the stiffness matrix. Thus the force vector is computed from stored element level values φ and c^{β} at the previous time step independently for each element. In contrast, the right-hand side for the finite element method (van Loon et al., 2003) is computed at the global level, requiring the multiplication of the entire stiffness matrix. Therefore the finite element method needs more CPU time due to the size of the matrices involved.

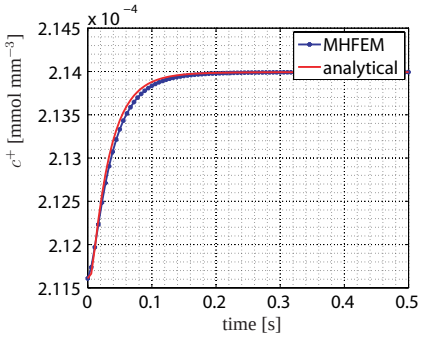
In conclusion, for the large problems for which a three-dimensional geometry is considered, the hybrid method offers significant advantages in both the amount of storage required and the CPU time to obtain a solution.



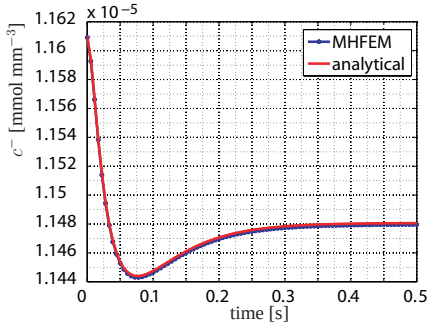
(a) μ^+ at $y = L$



(b) μ^- at $y = L$

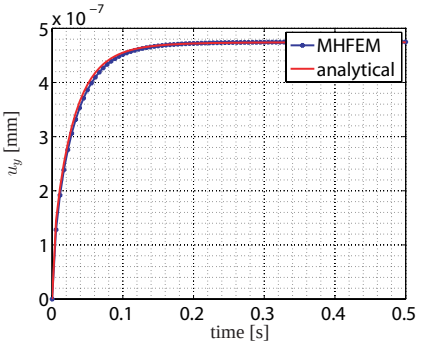


(c) cation concentration at $y = L$

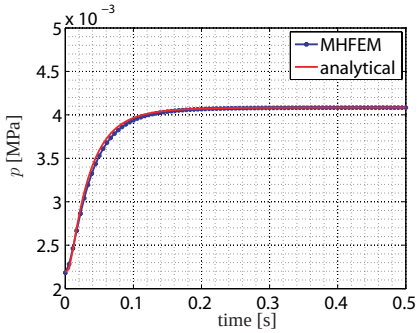


(d) anion concentration at $y = L$

Figure 5.3. Analytical-MHFEM comparison of the solutions for the confined consolidation (II).

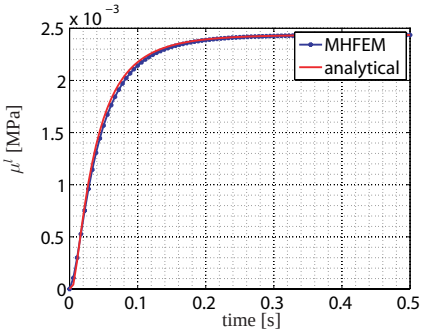


(a) Displacement at $y = L$

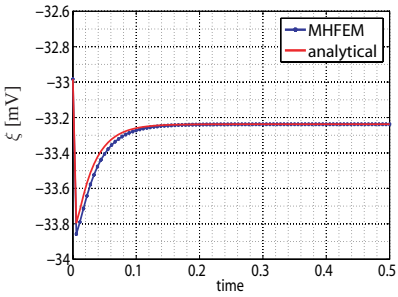


(b) Pore pressure at $y = L$

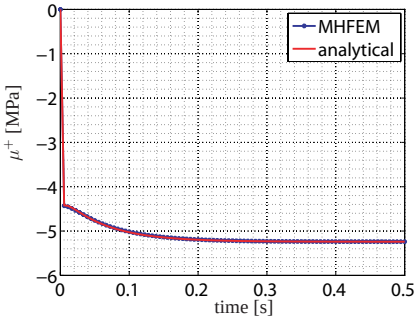
Figure 5.4. Analytical-MHFEM comparison of the displacement and pore pressure for confined swelling (I).



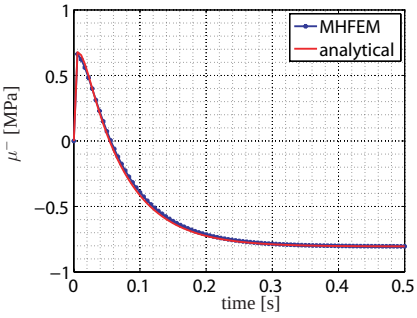
(a) μ^l at $y = L$



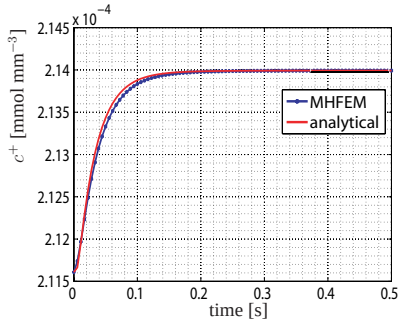
(b) electrical potential at $y = L$



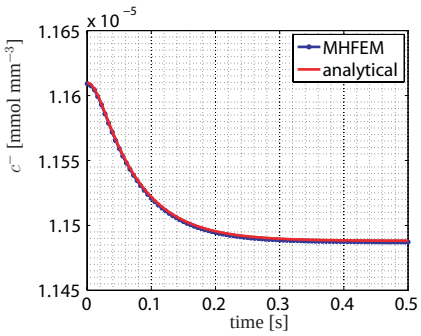
(c) μ^+ at $y = L$



(d) μ^- at $y = L$



(e) cation concentration at $y = L$



(f) anion concentration at $y = L$

Figure 5.5. Analytical-MHFEM comparison of the displacement and pore pressure for confined swelling (II).

5.3.2 Two-dimensional free swelling

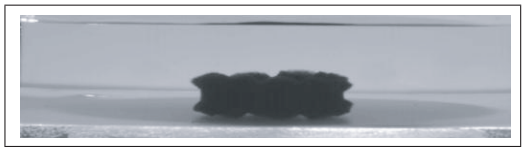


Figure 5.6. Experiment on hydrogel disc (J. M. Huyghe, 1999)

In this section, a mixed hybrid finite elements for two-dimensional four-component model is developed.

We consider the swelling cylinder to test the two-dimensional hybridization method. We choose an axisymmetric geometry as described below.

A cylinder of height 0.5 mm and radius 1 mm is in equilibrium with an external salt solution. The external concentration is reduced from 4.6×10^2 mol m^{-3} to 4×10^2 mol m^{-3}. A change of the salt concentration of this solution generates a change at the boundary of ion concentrations and electro-chemical potentials as well as pressure and voltage.

For this computation we take $\mu_s = 0.4688$ MPa, $\lambda_s = 0.3125$ MPa, $\varphi^f = 0.7$ and the other parameters are unchanged.

The intersection of the cylinder through the center is made in order to illustrate the swelling. For the boundary conditions of this rectangular shape intersection, we consider no horizontal displacement at the bottom left corner and no vertical displacement in the bottom. The bottom and top plane are considered impermeable. While the external salt concentration is reduced, the cylinder starts to shrink at the top surface where the salt concentration and the medium are in contact. This is due to the fact that the ions need less time to diffuse than the liquid, therefore an ions flow takes the liquid out of the sample and shrinkage happens. Further, the computation shows that after 6 hours the cylinder has regained its initial shape, however it is enlarged. Figure 5.7 shows the shrinkage period and following swelling period at the side surface.

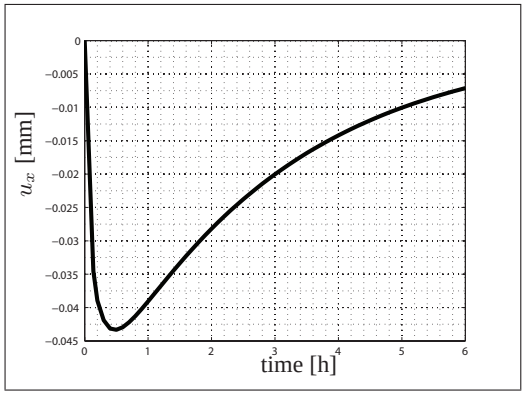
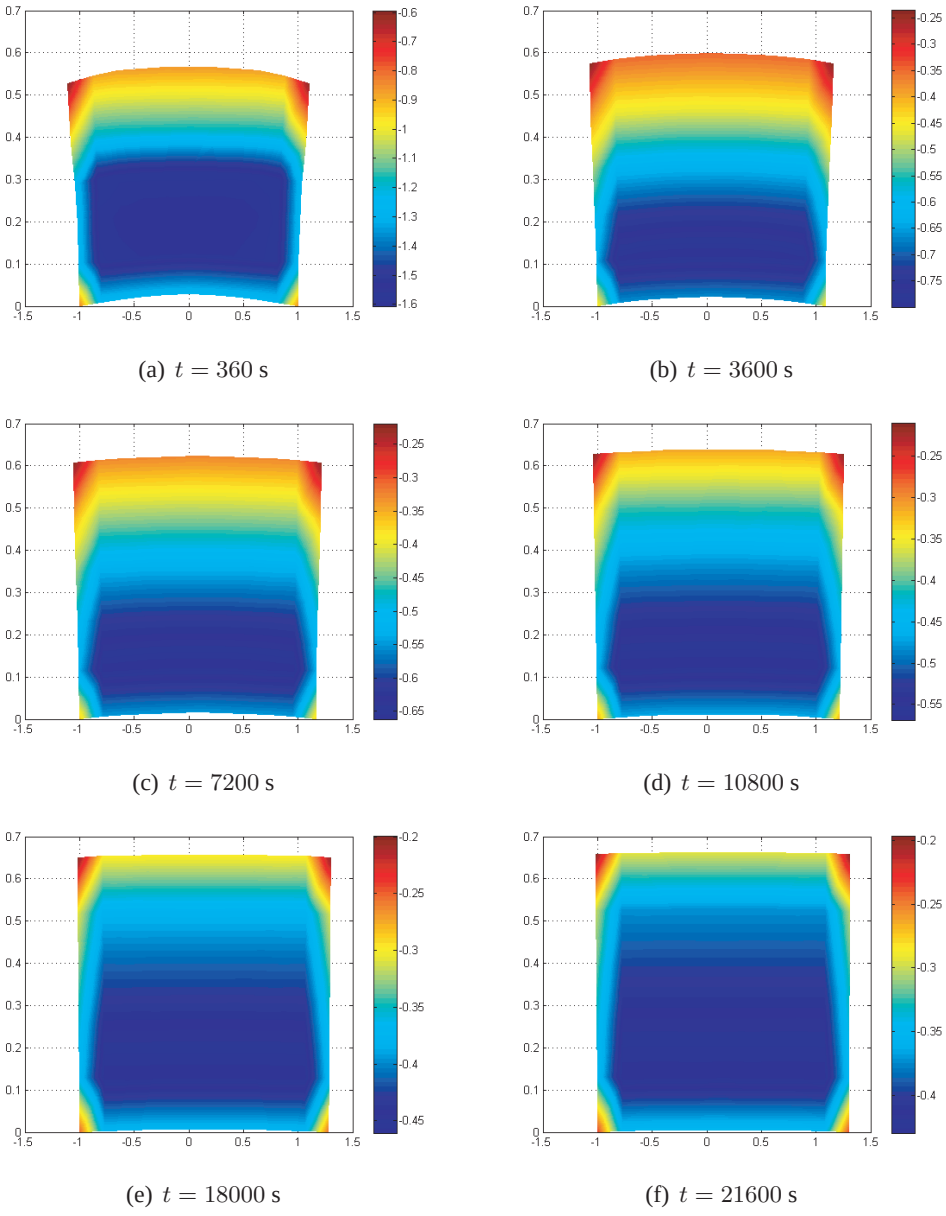


Figure 5.7. u_x on the top right point.

As it was expected for the higher dimensional geometry the number of iterations for the nonlinear solver is larger in comparison with the one-dimensional case. But thanks to the hybridization technique for less amount of storage it requires. Note that the nonlinear solver takes more iterations for the period ions are diffusing (the shrinkage period), later on while the hydrogel returns to its initial shape, the number of iterations is reduced to one iteration near final time.

Figure 5.8 (a-f) displays the swelling at different times.



(a) $t = 360$ s (b) $t = 3600$ s

(c) $t = 7200$ s (d) $t = 10800$ s

(e) $t = 18000$ s (f) $t = 21600$ s

Figure 5.8. Fluid pressure at intersection of cylinder for several times.

5.3.3 Opening cracks in the intervertebral disc

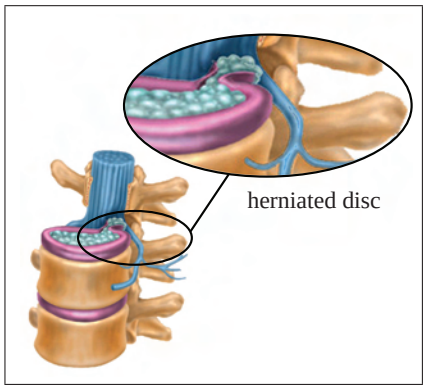


Figure 5.9. Schematic of a herniated disc

Low back pain is common in today's society. Seventy-five percent of all people will experience back pain at some time in their lives. Some of the common causes of back problems are disc injury (e.g., herniation and internal disc disruption) and degenerative discs.

The intervertebral disc serves as a shock absorber, load distributor and spacer. As we age the disc normally undergoes degenerative change. The disc loses its ability to hold water, resulting in decreased ability to absorb shock and a narrowing of the nerve openings in the sides of the spine, which may pinch the nerves. The result is increased disc stiffness often accompanied by back and leg pain.

The loss of proteoglycan in degenerate discs has a major effect on the disc's load-bearing behaviour. With loss of proteoglycan (and therefore fixed charges), the osmotic pressure of the disc falls and the disc is less able to maintain hydration under load; degenerate discs have a lower water content than normal age-matched discs, and when loaded they lose height and fluid more rapidly, and the discs tend to bulge.

Disc herniation occurs when the annulus fibrous breaks open or cracks, allowing the nucleus pulposus to escape. This is called a Herniated Nucleus Pulposus (HNP) or herniated disc.

A herniated lumbar disc can press on the nerves in the spine and may cause pain, numbness, tingling or weakness of the leg called "sciatica". Sciatica affects about 1-2 $\%$ of all people, usually between the ages of 30 and 50.

A herniated lumbar disc may also cause back pain, although back pain alone (without leg pain) can have many causes other than a herniated disc.

In (Wognum et al., 2006) the influence of decreasing osmotic pressure on the opening of cracks in the intervertebral disc is studied, both experimentally and numerically. The numerical solutions are derived from finite element method, assuming displacement, fluid pressure, electro-chemical potentials, electrical potential and volume fractions to be unknowns.

In our work, we consider the mixed finite element formulation with the hybridization technique. In fact, the mixed variational method has been shown to be suitable for this kind of problem, when a crack tip is considered inside the domain. The mixed method owes its popularity to its local (element-wise) mass conservation property and the simultaneous and accurate approximation of variables of physical interest, e.g., potentials and flows. The mixed method for the four-component model has less number of unknowns by using the hybridization technique and is stable near the crack tips. We consider a two-dimensional rectangular geometry 2×0.5 mm with a 1 mm long crack in the center as it is described in Figure 5.10.

The up and bottom of the sample are fixed, the left side and the crack can move freely. We assume that initially the crack is closed at equilibrium with the external

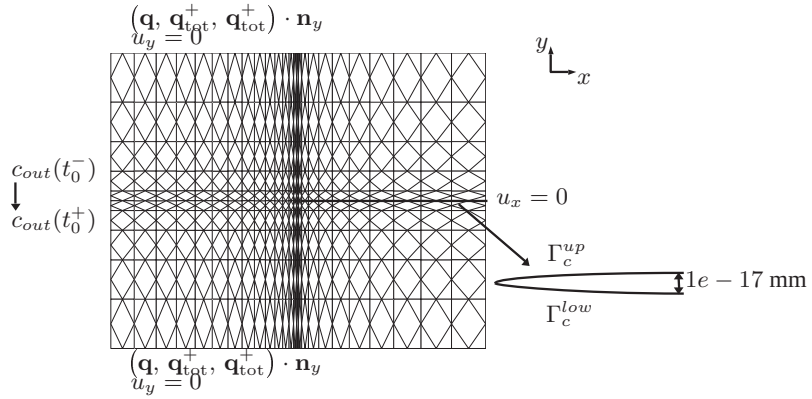


Figure 5.10. Schematic representation of the crack problem.

bathing solution with concentration $c_{out}(t_0^-) = 1.5 \times 10^2$ mol m^{-3}. At $t = t_0^+$, the concentration of the external solution at the left side of sample increases to $c_{out}(t_0^+) = 2 \times 10^2$ mol m^{-3} instantaneously (Wognum et al., 2006).

The following parameters are taken:

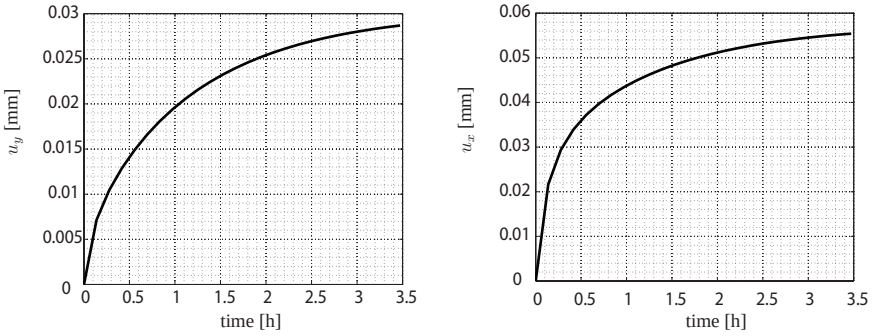
Parameter	Unit	Value
$2\mu_s + \lambda_s$	MPa	1
K	m^4 N^{-1} s^{-1}	0.28×10^{-15}
c^{fc}	mol m^{-3}	-2×10^2
c_{out}	mol m^{-3}	1.5×10^2
φ		0.8
D^+	m^2 s^{-1}	13.3×10^{-10}
D^-	m^2 s^{-1}	20.3×10^{-10}
R	J mol^{-1} K^{-1}	8.3145
T	K	298
F	C mol^{-1}	96484.6
Γ		0.9

Table 5.1. Material parameters

Figure 5.11 shows the displacement changes for both crack top point and the left side of the domain. The numerical simulations for the opening crack are shown in Figure 5.12.

5.4 Conclusions and future directions

Assuming infinitesimal deformation for the solid phase, four-component modelling of biological tissues is derived in chapter 2. This results in a coupled system of non-linear parabolic differential equation. For the numerical experiments it is clear that an accurate approximation of the flows can be determined by the mixed finite element method. The benefit of the mixed method are apparent for problems with rough



(a) uy at top crack (b) u_x at left side

Figure 5.11. Displacement for the top crack and left side.

tensors of hydraulic conductivity (for example confined compression and swelling method) and especially if the domain is subdivided into very flat sub-domains.

Of course, if one is interested in an accurate approximation of the potential, then the conforming finite element is preferable with a non-uniform time discretisation with a larger steps near the equilibrium. The number of required iterations to solve the nonlinear system is reduced for one-dimensional experiments.

Using the hybridization technique, the mixed finite element method still results in an indefinite system but will less number of degrees of freedom. We use iteration for solving the nonlinear system derived after taking the Backward Euler scheme for the time integration. This algorithm has been tested for one-dimensional confined consolidation and free swelling experiment and the results has been verified with analytical solutions.

A two-dimensional swelling and opening crack problem is tested by using hybridization method. Note that for higher dimensional problem we are aware of using an iterative solver to solve the system of equations. even more a right preconditioner is needed for our indefinite system. The implicit time discretisation is unconditionally stable, but still we should be careful in choosing the time step to avoid possible oscillations.

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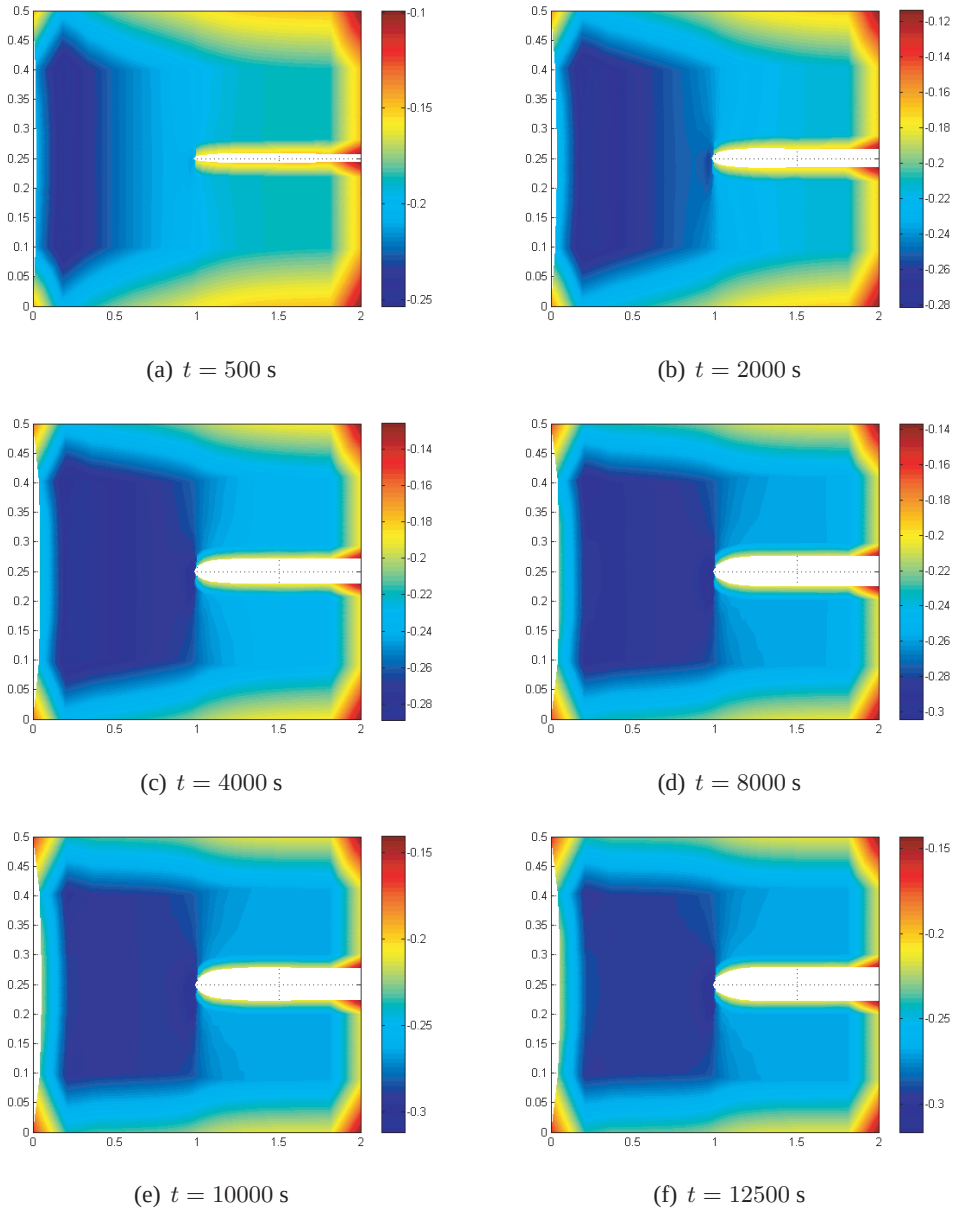

(a) $t = 500$ s (b) $t = 2000$ s

(c) $t = 4000$ s (d) $t = 8000$ s

(e) $t = 10000$ s (f) $t = 12500$ s

Figure 5.12. Fluid pressure for opening crack problem at several times.

Summary

Mixed Finite Element for Swelling of Cartilaginous Tissues

Many biological porous media exhibit swelling and shrinking behaviour when in contact with salt concentrations. This phenomenon, observed in cartilage and hydrogel, is caused by electric charges fixed to the solid, counteracted by corresponding charges in fluid. These charges result in a variety of features, including swelling, electro-osmosis, streaming potentials and streaming currents.

Mixture theory is a framework, in which the model integrates mechanical deformations, loads, diffusion, convection and chemical reactions of different solutes.

An earlier study from geomechanics presents biphasic models that describe the solid-fluid interactions. These models cannot describe osmotic effects that have major influence on the behaviour of tissues. Therefore to account for osmotic effects this is modelled by a four-component mixture theory.

In the four-component mixture theory a deformable and charged porous medium is saturated with a fluid with dissolved cations and anions. Four components are defined: solid, liquid, cations and anions. Balance equations for each component as well as for the mixture are given. Together with the second law of thermodynamics, the constitutive equations are given.

This theory results in a coupled system of nonlinear parabolic differential equations together with an algebraic constraint for electroneutrality.

In this model, it is desirable to obtain an accurate approximation of the fluid and ions flow. Such an accurate approximation can be determined by the mixed finite element method.

We consider the numerical solution of the mentioned problem using a mixed discretisation by Raviart-Thomas-Nédélec elements on two- and three-dimensional domains.

The solid displacement, fluid and ions flow and electro-chemical potentials are taken as degrees of freedom. This results into a first-order nonlinear algebraic equation with an indefinite coefficient matrix.

The hybridization technique is then used to reduce the list of degrees of freedom and to speed up the numerical computations.

The mixed hybrid finite element method is validated for small deformations using analytical solutions for one-dimensional confined consolidation and swelling. Two-dimensional results are shown for a swelling cylindrical hydrogel sample and opening cracks in intervertebral disc.

Samenvatting

Veel biologische poreuze media vertonen zwel- en krimpgedrag wanneer deze in contact komen met zoutoplossingen. Dit fenomeen, dat in kraakbeen en hydrogel wordt waargenomen, wordt veroorzaakt door elektrische ladingen die aan de vaste stof gebonden zijn, die door overeenkomstige ladingen in de vloeistof worden tegengewerkt. Deze ladingen resulteren in een verscheidenheid van verschijnselen, met name zwelling, electro-osmose, stromingspotentialen en elektrische stromingen.

De mengseltheorie is een raamwerk, dat mechanische deformaties, ladingen, diffusie, convectie en chemische reacties van verschillende opgeloste stoffen integreert.

Een eerdere geomechanische studie stelt tweefasenmodellen voor, die de interactie beschrijven tussen vaste stof en vloeistof. Deze modellen kunnen osmotische effecten, die een belangrijke invloed op het gedrag van weefsels hebben, niet beschrijven. Daarom wordt dit gemodelleerd met de vier-componentenmengseltheorie om osmotische effecten te beschouwen.

In de vier-componentenmengseltheorie is een vervormbaar en geladen poreus medium verzadigd met een vloeistof met opgeloste kationen en anionen. Vier componenten worden gedefinieerd: vaste stof, vloeistof, kationen en anionen. De balanswetten voor elke component evenals voor het mengsel worden gegeven. Samen met de tweede wet van de thermodynamica worden de constitutieve vergelijkingen gegeven.

Deze theorie resulteert in een gekoppeld stelsel niet-lineaire parabolische differentiaalvergelijkingen tezamen met een algebraïsche voorwaarde voor elektroneutraliteit.

In dit model is het wenselijk om een nauwkeurige benadering van de vloeistof- en ionenstroom te verkrijgen. Een dergelijke nauwkeurige benadering kan worden verkregen met behulp van de gemengde eindige elementenmethode.

We beschouwen de numerieke oplossing van het bovengenoemde probleem gebruikmakend van gemengde discretisatie met Raviart-Thomas-Nédélec elementen op twee- en driedimensionale domeinen.

De deformatie, vloeistof- en ionenstroom, en de elektrochemische potentiaal worden genomen als graden van vrijheid. Dit resulteert in een eerste orde niet-lineaire algebraïsche vergelijking met een indefiniete coëfficiëntenmatrix.

De hybridisatietechniek wordt vervolgens gebruikt om de lijst vrijheidsgraden te verkleinen en de numerieke berekeningen te versnellen.

De gemengdhybride eindige elementenmethode wordt voor kleine vervormingen

gevalideerd met hulp van analytische oplossingen voor eendimensionale beperkte consolidatie en zwelling. Tweedimensionale resultaten worden getoond voor een monster van zwellende cilindrische hydrogel en het openbarsten in de tussenwervelschijf.

چکیده

روش اجزاء محدود آمیخته هیبریدی برای تورم بافتهای غضروفی

بسیاری از مواد متخلخل بیولوژیکی در مجاورت محلول نمك متناسب با غلظت نمك رفتارهای تورمی و انقباضی از خود نشان می دهند. علت این پدیده که در نرمه استخوان (غضروف) و هیدروژل مشاهده می شود، تقابل یونهای ساکن در اسکلت جامد با یونهای نظیر در سیال می باشد. وجود این یونها یکسری از خواص ازجمله تورم، نفوذ الکتریکی (الکترو اسمزی)، پتانسیلهای جریانی و جریانهای الکتریکی را نتیجه میدهد.

نظریه آمیزه در حقیقت چهار چوبی است که درآن بار و تغییر شکل مکانیکی، انتشار، انتقال و واکنشهای شیمیایی حلالهای متفاوت درآن مطالعه می شود.

در مطالعات اولیه ژئومکانیك مدلهای دو فازی را می توان یافت که اندرکنش جامد و سیال درآنها آمده است. در حقیقت این مدلها قادر به در نظر گرفتن اثرات اسمزی یونها که تاثیر بسزایی بر رفتار بافتها دارند نیست. ازاینرو نظریه چهار مولفه ای آمیزه برای در نظر گرفتن این تاثیرات مورد مطالعه قرار می گیرد.

در نظریه چهار مولفه ای آمیزه یك ماده متخلخل شکل پذیر و یونیزه با یك سیال که در آن یونهای مثبت و منفی حل شده اند اشباع می شود. در این مدل چهار مولفه تعریف می شود: جامد، مایع، یونهای مثبت و یونهای منفی. معادلات توازن برای هر یك از مولفه ها و برای آمیزه در نظر گرفته می شود. با استفاده از قانون دوم ترمودینامیك معادلات مشخصه نیز ارائه می شود.

در نهایت این نظریه یك سیستم غیر خطی از معادلات دیفرانسیل با مشتقات جزئی سهموی بهمراه یك قید جبری برای خنثی سازی الکتریکی بدست می دهد.

هدف اصلی در این مدل محاسبه تقریبی شارسیال و شار یونها با دقت کافی میباشد. چنین تقریبی رامیتوان با استفاده از روش اجزاء محدودآمیخته بدست آورد. جواب های عددی مدل ذکر شده بالا با استفاده از روش گسسته سازی آمیخته و با در نظر گرفتن المانهای راویارت-توماس- نِدِلِك برای دامنه های دو و سه بعدی محاسبه می شوند.

تغییر مکان اسکلت جامد، شار مایع و یونها و پتانسیلهای الکترو شیمیایی به عنوان درجات آزادی سیستم در نظر گرفته می شوند. در نتیجه یك معادله غیر خطی جبری با یك ماتریس ضرایب نامعین خواهیم داشت.

تکنیك هیبریداسیون برای کاستن از تعداد درجات آزادی و افزایش سرعت محاسبات عددی استفاده میشود.

جوابهای بدست آمده از روش اجزاء محدود آمیخته هیبریدی با جوابهای تحلیلی در حالتیکه تغییر شکل فاز جامد بسیار کوچك فرض شده باشد برای مسائل تحکیم و تورم محدود شده سنجیده میشوند. نتایج در حالت دو بعدی برای تورم آزاد یك نمونه استوانه ای شکل از هیدروژل و مساله باز شدن ترك در دیسك بین مهره ها نشان داده می شود.

Curriculum Vitae

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