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Development of a new non-linear elastic hydro-mechanical model for the simulation of compacted MX-80 bentonite: application to laboratory and *in situ* sealing experiments for geo-repository engineered barriers.

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Abstract

The management of radioactive wastes is a significant environmental issue facing the international nuclear community today. The current international consensus is for disposal of higher activity waste from a variety of sources in deep geological disposal facilities (GDFs). Hydraulic seals, often planned to consist of compacted bentonite-sand blocks, are an important part of the closure phase of a GDF. As such, an understanding of the hydro-mechanical (HM) behaviour of these seals, and the ability to model and predict their behaviour is fundamental to support many planned safety cases and licence applications. Bentonite is well suited for use as a hydraulic seal due to its high swelling capacity that enables it to swell into voids while maintaining a low permeability sealed barrier to advective flow, and to provide structural support by generating a swelling pressure on the excavation walls.

The hydro-mechanical process of bentonite hydration is a highly non-linear problem. As such, coupled process models that are able to account for the strong inter-dependence of the hydraulic and mechanical processes are employed to simulate the behaviour of bentonite under repository conditions. This thesis reports the development of an HM coupled model in the open source finite element code OpenGeoSys (OGS), and its application to the simulation of a range of hydraulic seal test conditions.

The developed model couples Richards' equation for unsaturated flow to a new strain dependent non-linear elastic mechanical model that incorporates a Lagrangian moving finite element mesh to inform the material non-linearity. Stress and volumetric dependent water retention behaviour are incorporated through the implementation of the Dueck suction concept extended to take into account non-recoverable strains during consolidation. A number of permeability functions are implemented and tested against experimental data.

The mechanical model is extended to account for wetting-induced collapse behaviour by the definition of a failure curve derived from experimental results. Similar in definition to the Loading-Collapse curve in elasto-plastic models, this failure curve triggers the application of a source term to account for wetting-induced collapse.

Coupling between the hydraulic and mechanical processes is achieved through the stress dependency of the water retention behaviour, the inclusion of a new coupling factor for the hydraulic contribution to the mechanical process, and the dependency of numerical convergence criteria on net mean stress. An explicit iterative calculation approach is employed. As a result, the hydraulic and mechanical moving meshes are decoupled to allow volumetric dependent parameters to be updated within process iterations.

The model is calibrated and compared to experimental data from the SEALEX experiments conducted by the Institut de Radioprotection et de Sûreté Nucléaire (IRSN) at the Tournemire URL, France. The experimental programme comprises standardised laboratory tests, a $1/10^{th}$ scale mock-up of a hydraulic seal with a uniform technological void, and a full scale *in situ* performance test with a non-uniform technological void due to its horizontal geometry.

Using a model with 5 hydraulic parameters, 8 mechanical parameters with an experimentally defined failure curve, and one coupling parameter, the major trends of behaviour in all the SEALEX experiments can be recreated, including axial stress build up, water uptake, and final deformation. However, the elastic method employed leads to an over prediction of the rebound on loss of axial confinement in the $1/10^{th}$ scale mock-up test.

Simulations suggest that the non-symmetric technological void in the full scale performance test could have lasting effects on the development of heterogeneity in the hydraulic seal. The development of heterogeneity does not adversely affect the permeability with respect to the design criteria, but may have significant consequences for the development of a heterogeneous swelling pressure.

Lay Summary

Waste products from defence activities, medical and industrial applications, and the generation of nuclear power, can contain radioactive elements. The safe management of this waste is a major challenge facing the international community. One option favoured by many countries that have radioactive waste, is to package it up in specially design containers/canisters and dispose of it in an underground facility in the rock, known as a Geological Disposal Facility (GDF). Waste packages will be placed in tunnels and holes in the facility and then sealed to prevent movement of waste out of the facility. The combination of the specifically designed waste packages, the sealing material, and the host rock is known as the multi-barrier approach and aims to isolate and contain the waste.

Rocks in and around a GDF are likely to contain water that can gradually flow through tiny space in the rock known as pores. Water flowing through the disposal facility has the potential to transport any waste that may escape from the specially designed waste packages, so many plans for a GDF involve a method to slow and inhibit water flow to and from the waste packages. One method of inhibiting flow is through the use of a sealing material in a hydraulic seal device.

The ability of water to flow through a rock is measured by its permeability, so a sealing material is designed to have a very low permeability. One material under consideration is a clay called bentonite. It has a very low permeability but it also has the special property that it swells when in contact with water. This is caused by the minerals in the clay attracting and absorbing water, which causes an increase in volume. This attractive force is known as suction as it 'sucks' up water into the clay, and is an active force until no more water can enter the sample i.e. until it becomes saturated.

Gaps may exist between the clay sealing device and the rock due to reasons of practicality during the insertion of the hydraulic seal. Therefore, bentonite's swelling potential allows it to provide an effective seal by swelling to fill all possible spaces while maintaining a low permeability barrier. The aim of this is to return the excavated tunnel or borehole to a state that has similar (or more advantageous) properties to the surrounding rock.

Once all the gaps have been filled by the swelling bentonite, additional water flowing to or from the waste packages may continue to flow into the bentonite if it is not fully saturated. Although flow is extremely slow, the increase in water content leads to a build up of pressure within the clay (known as the swelling pressure), which exists because the sample wants to, but cannot expand any further. This swelling pressure pushes out against the rock and provides support to the excavated tunnel or borehole walls. When designing a hydraulic seal, the key criteria are the low permeability and the swelling pressure. It is therefore important to have a good understanding of the processes of how the water flows through bentonite, how the bentonite swells, and how much swelling pressure will be generated.

Experiments are commonly used to investigate and improve understanding of bentonite behaviour in conditions similar to those expected in a disposal facility. However, radioactive waste can be extremely long-lived, so a disposal programme needs to demonstrate an adequate level of safety for a time period upwards of 1,000,000 years. Consequently, a full 'dry run' experiment is not possible and numerical modelling is required to predict the long term behaviour of the components of a disposal system. Numerical models are developed alongside experiments that can be considered long-term by human standards e.g. 5-20 years, in order to build confidence that the model is representing processes that are happening in the hydraulic seal.

This project reports the development of a numerical model that is used to simulate the behaviour of the hydraulic seal material in both laboratory experiments and full scale *in situ* performance tests performed as part of the French regulator's research and development program for radioactive waste disposal. The experimental programme investigated the effect of gaps (known as technological voids) on the sealing behaviour of a bentonite hydraulic seal.

The model is first shown to recreate results from small scale lab experiments before being applied to a full-scale *in situ* performance test. Model simulations of the full scale performance test showed that the permeability of the seal is within the design criteria, but a non-uniform technological void around the clay sealing device could lead to a variation in swelling pressure

development as a result of different amounts of swelling experienced by the bentonite. The process of developing this variability needs to be well understood as swelling pressure is one of the main design criteria for hydraulic seals.

Declaration and attribution of work

I declare that this thesis has been composed by myself and that it has not been submitted, either whole or in part, in any previous application for a degree. Except where otherwise acknowledged, the work presented is my own.

Andrew Fraser Harris

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List of Symbols

In addition to the symbols listed here, the symbols x , y , and z have been used throughout to denote the cartesian coordinate axes.

Symbol	Description	Units
a, b, c, d	Empirical parameters to fit the free swell suction curve [Bond and Benbow, 2009]	-
a_p	Specific surface area per unit volume of particles in the Kozeny-Carmen equation	m^2
A	Area	m^2
$A_p(s)$	Void ratio when mean stress (p) is equal to a reference stress (p_c) ([Cui et al., 2002])	-
$A_s(p)$	Void ratio when suction (s) is equal to a reference suction (s_c) ([Cui et al., 2002])	-
$\text{\AA}$	Angstrom unit of distance	
$\mathbf{b}$	Vector of body forces in mechanical model	Pa
$\mathbf{B}$	Strain displacement matrix	
$C(\psi)$	Specific moisture capacity	
$C(s)$	Correction Factor in Fredlund and Xing [1994] water retention function	-
d	Dimensionality factor in new non-linear elastic model	-
$D^{(e)}$	Elastic constitutive matrix	Pa
e	Void ratio	-
e_0	Initial void ratio	-
e_m	Micro-structure void ratio	-
e_M	Macro-structure void ratio	-
$ err $	Error criterion for coupling procedure	Pa
E	Elastic modulus	Pa
E_{min}	Minimum E threshold in new non-linear elastic model	Pa
E_t	Elastic modulus at time t	Pa
$\mathbf{F}$	Flux vector in the hydraulic solution	m^3/s
$\mathbf{f}$	Force vector in the mechanical solution	Pa
F	Failure ellipsoid in the Cam Clay model	
$f_{I0}, f_{I1}, n_I, f_{D0}, f_{D1}, n_D$	Fitting parameters for BExM interaction function	
g	Acceleration due to gravity	m/s^2
h	Air pressure in Brooks and Corey [1964] model	Pa
h_e	Air entry pressure in Brooks and Corey [1964] model	Pa
i	Hydraulic gradient	-
J	Jacobian transformation matrix	-

Symbol	Description	Units
k	Intrinsic permeability	m^2
k_{rel}	Relative permeability	
k_{red}	Reduction factor in calculation of E below E_{min}	
k_0	Pore shape factor in Liu et al. [2011] permeability model	
K	Hydraulic conductivity	m/s
$[K]$	Stiffness matrix	
l	Exponent in Liu et al. [2011] permeability model	
L	Differential operator for mechanical solution	
L	Length	m
m	van Genuchten parameter	
m_a	Exponent in Liu et al. [2011] permeability model	
m_s	Mass of solids	kg
M	Slope of the critical state line	
M_b	Mass fraction of bentonite	
M_w	Gravimetric water content	-
$M_{w_{max}}$	Max gravimetric water content	-
n	Porosity	-
n_v	van Genuchten parameter	
$N_i^{(e)}$	Interpolation function at node i in element (e) . Subscripts j and k are used for other nodes	
N_{i*}	Interpolation function for the time derivative in a lumped element formulation	
$N_p(s)$	Slope of data in a $\log(p):\log(e)$ plot in Cui et al. [2002]	
$N_s(p)$	Slope of compression index in a $\log(p):\log(e)$ plot at constant suction Cui et al. [2002]	
p	Mean net stress	Pa
p_{atm}	Atmospheric pressure	Pa
p_c	Reference stress in Cui et al. [2002]	Pa
$p_{c\alpha}$	Capillary pressure of phase α	Pa
p_{con}	Pre-consolidation pressure	Pa
p^*_0	Saturated yield stress in the BBM	Pa
q	Deviatoric stress	Pa
q_α	Darcy flux of phase α	m/s
Q	Volumetric flow rate	m^3/s
Q_α	Source term in the unsaturated flow equation	m^3/s
r_m	Maximum stiffness a soil could reach (in BBM)	Pa
r	Radius	m
R	Gas constant	$\text{J mol}^{-1}\text{K}^{-1}$
$R_i^{(e)}$	Residual at node i in element (e) . Subscripts j and k are used for other nodes	
RH	Relative humidity	%

Symbol	Description	Units
s	Suction pressure	Pa
s_c	Reference suction in Cui et al. [2002]	Pa
s_{fs}	Free swell suction	Pa
s_m	Matric suction	Pa
s_{net}	Net suction	Pa
s_r	Suction at residual saturation	Pa
S	Saturation	%
$S_{t\alpha}$	Storativity of phase α	-
S_α	Saturation of phase α	%
S_e	Effective saturation	%
ST	Applied source term in NLE-ST model	Pa
T_k	Temperature in degrees Kelvin	K
$\mathbf{u}$	Displacement vector	m
u_{max}	Maximum displacement for boundary conditions	m
u_a	Air pressure	Pa
u_v	Partial pressure of water vapour	Pa
u_{v0}	Saturation pressure of pure water	Pa
u_w	Fluid pressure (water)	Pa
v	Fluid velocity	m/s
v^r	Recoverable volume (Cam Clay model)	m ³
v_a	Specific volume of sample	m ³
v_{w0}	Specific water volume	m ³
V_t	Element volume	m ³
V_a	Volume of air	m ³
V_v	Volume of voids	m ³
V_w	Volume of water	m ³

Greek Symbols	Description	Units
α	van Genuchten parameter	-
α_w	Fitting parameter in Wang [2012] dry density-swelling relationship	-
α_h, α_s	Strain hardening and softening parameter in new non-linear elastic model	-
α_k	Fitting parameter in Karnland et al. [2006] permeability model	-
α_B	Biot's constant	-
β_w	Fitting parameter in Wang [2012] dry density-swelling relationship	-
β_k	Fitting parameter in Karnland et al. [2006] permeability model	-
β_s	Parameter controlling the rate of increasing stiffness with suction in BBM	-
γ	Shear strain	-
γ_v	van Genuchten parameter	-
Γ	Denotes a surface over-which integration is performed	-
δ_p	Average montmorillonite sheet thickness in Liu et al. [2011] model	nm
ϵ	Strain	-
ϵ_v	Volumetric strain	-
ϵ^e	Elastic strain	-
ϵ^p	Plastic strain	-
ϵ_v	van Genuchten parameter	-
ζ_p	Mass fraction of montmorillonite with respect to the solids	%
η	Exponent of relative permeability	-
θ_{res}	van Genuchten parameter for residual water content	-
θ_s	van Genuchten parameter for saturated water content	-
θ_w	van Genuchten parameter for measured/calculated water content	-
Θ	Volumetric water content	%
ι	Third stress invariant	-
κ	κ -line in the Cam Clay model and BBM	-
λ	The slope of the virgin consolidation curve in the Cam Clay model	-
$\lambda(s)$	The slope of the virgin consolidation curve dependent on suction	-
$\lambda(0)$	The slope of the virgin consolidation curve at saturation	-
λ_p	Pore size distribution factor	-
μ	Viscosity	Pa · s
ν	Poisson's ratio	-
ξ	Unknown point in time between time interval	-
π	Osmotic suction	Pa

Greek Symbols	Description	Units
ρ	Density	kg/m ³
ρ_α	Density of phase α	kg/m ³
ρ_d	Dry density	kg/m ³
ρ_{ref}	Reference density	kg/m ³
ρ_s	Density of solids	kg/m ³
σ	Stress	Pa
σ_c	Confining stress	Pa
σ_{th}	Threshold stress of failure curve	Pa
σ_v	Net axial stress	Pa
σ_H	Hydraulic stress	Pa
σ_M	Mechanical stress	Pa
σ_T	Total stress	Pa
σ'	Effective stress	Pa
σ''	Modified effective stress	Pa
τ	Shear stress	-
τ_a	Tortuosity factor	-
Υ	Internal strain factor	-
ϕ	Soil constant in Gallipoli et al. [2003] function	-
ϕ_k	Volume fraction of the solid	%
χ	Bishops parameter	-
ψ	Pressure head	Pa
ψ_g	Soil constant in Gallipoli et al. [2003] function	-
ω	Weighting function	-
ω_v	Molecular mass of water vapour	kg
ω_w	Molecular mass of water	kg
Ω	Denotes Area over-which integration is performed	-

Maths Symbols	Description
div	Divergence operator
$\cdot$	Denotes derivative of time
exp	Exponential function
$grad$	Gradient operator
$\hat{}$	Denotes approximated solution of field variable
I	Identity matrix
tr	Trace of the tensor

Chapter 1

Introduction

1.1 Background

Ever since its discovery by Antoine Henri Becquerel in 1896, radioactivity has been exploited by man for a wide variety of applications [Lowenthal and Airey, 2001]. It arises as a result of unstable isotopes emitting radiation in a process of radioactive decay. This process releases energy that can be exploited for applications such as medicinal procedures, research, and commercial electricity generation. For example, if the isotope is large e.g. U^{235} , and decays into unstable daughter isotopes which themselves decay, a chain reaction can be produced in which the emitted energy can be harnessed and controlled to produce usable energy i.e. electricity [Lowenthal and Airey, 2001]. An unfortunate by-product of the anthropogenic exploitation of radioactivity is the generation of concentrated, non-economic radioactive material which can contain long-lived radionuclides i.e. radioactive waste.

Consequently, the long term management of radioactive waste has become a significant topic of international research in the recent decades, especially as many of the world's nuclear power stations near the end of their operational lifetime and require decommissioning. Furthermore, it is expected that the nuclear legacy will not just amount to the current stock-piled wastes but include waste generated by future generations of nuclear power plants [Tweed et al., 2015]. The nuclear industry is expected to expand as countries facing carbon emission targets aim to decarbonize their energy portfolios and meet international agreements e.g. commitments recently pledged at COP21 in Paris.

One method of managing radioactive wastes is disposal that aims to contain it within a localised disposal facility where it is isolated from the biosphere. The mode of disposal of radioactive wastes varies with the waste type. Low activity material in the UK is disposed of in surface, or near surface facilities, but higher activity wastes are planned to be disposed of via deep geological disposal facilities (GDFs) [Kim et al., 2011, Tweed et al., 2015]. The need to provide safe long-term disposal has led to an intensive research effort, not only from the international research community, but also from companies and organisations responsible for disposal implementation and for the regulation of disposal. The product of these efforts is a large body of research stretching across many disciplines and aiming to cover all expected aspects of the proposed disposal systems and support license applications e.g. [Alonso et al., 2005, Barnichon et al., 2012, Gaus et al., 2014, NAGRA, 2009, Nguyen et al., 2005, Palacios et al., 2014, POSIVA, 2010, Rutqvist et al., 2005].

Currently, there are no operational GDFs for higher activity wastes, but a number of implementers have submitted licence applications e.g. Posiva Oy (Finland) and SKB (Sweden) [Kim et al., 2011, NDA, 2013]. Some lower activity waste materials have previously been disposed of in underground facilities such as the Waste Isolation Pilot Plant (WIPP) in the USA, and Asse II Mine, Germany with varying degrees of success, and a decision on the Canadian Deep Geological Repository (DGR) is expected by 1st of March 2016 [www.ceaa-acee.gc.ca]. In the case of Posiva Oy, their GDF licence application has recently proved to be successful with the world's first construction licence for higher activity waste disposal granted in November 2015 by the Finnish government [www.nda.gov.uk]. Other disposal programmes are currently engaging in public consultations and active research with the view to submit licence applications in the near future e.g. the French and Swiss programmes led by the French National Radioactive Waste Management Agency (ANDRA) and the Swiss National Cooperative for the Disposal of Radioactive Waste (NAGRA) respectively.

1.1.1 Radioactive Waste Disposal

Radioactive waste can be produced either through direct sources such as spent nuclear fuel and the production of radioactive daughter elements, or indirectly via neutron bombardment. As a result radioactive waste comes in many forms with different properties, and the subsequent management requires different approaches for different wastes [NIREX, 2002]. The main sources of such wastes are commercial electricity production, subsequent decommissioning of nuclear power plants, defence related activities, and, to a lesser extent, medicine and research activities [Tweed et al., 2015]. In the UK wastes are classified according to their nature and level of radioactivity and potential for heat generation by continual decay, as outlined in Table 1.1 [NDA, 2010].

In addition to the waste classification system in Table 1.1, UK radioactive materials are also

Very Low Level Waste (VLLW)	VLLW is not considered in the UK waste inventory as it refers to wastes that can be disposed of in normal refuse and control only needs to be exercised if the large volumes are disposed in one particular location [NIREX, 2002].
Low Level Waste (LLW)	".... wastes having a radioactive content not exceeding 4 gigabecquerels (GBq) per tonne of alpha, and 12 GBq of beta/gamma activity" [NDA, 2010]
Intermediate Level Waste (ILW)	"... wastes exceeding the upper boundaries for of the LLW but which do not require heating to be taken into account in the design of storage or disposal facilities" [NDA, 2010]
High Level Waste (HLW)	"... Wastes in which the temperature may rise significantly as a result of their radioactivity, so this factor has to be taken into account in the design of storage or disposal facilities" [NDA, 2010]
Spent Fuel (SF)	Spent fuel is not currently classified as waste as it could potentially be reprocessed and recycled for further use. In the future in the UK it is anticipated that spent fuel will be subject to direct disposal as is planned in other countries e.g. Finland [POSIVA, 2010, Tweed et al., 2015]

Table 1.1: Categories of radioactive wastes in the UK waste inventory 2010 [NDA, 2010]

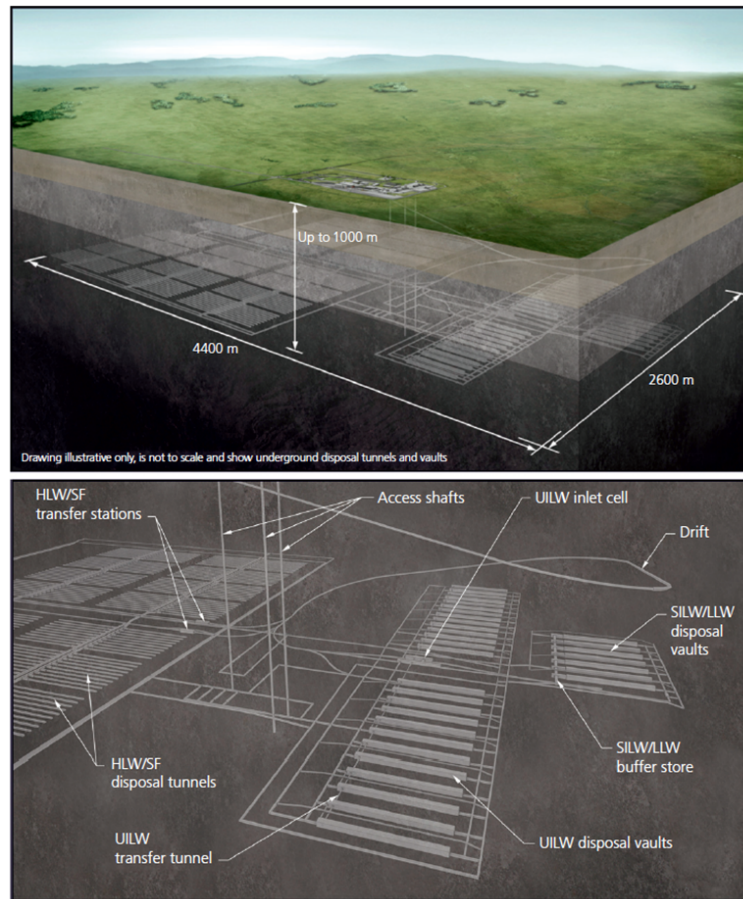


Figure 1.1: Schematic diagrams showing a generic concept for deep geological disposal after Tweed et al. [2015]. The disposal facility at depth is divided into separate regions containing different types of radioactive waste depending on their classification as HLW, ILW, LLW, or SF.

classified by their disposal requirements. Wastes are classified depending on whether they can be disposed of in a surface, near surface facilities, or if they require deep geological disposal [Tweed et al., 2015]. Geological disposal is proposed for all Higher Activity Wastes (HAWs) which include High Level Waste (HLW), Intermediate Level waste (ILW), some Low Level Waste (LLW) that cannot be disposed of in surface facilities, and spent fuel (SF) from current, and future, commercial power generation [Tweed et al., 2015]. Consequently, under this classification system a GDF could potentially be a combined HLW and ILW repository with separate disposal areas for heat generating and non-heat generating wastes (Figure 1.1). The specific needs for disposal in each section of the repository are defined by the waste category e.g. heat generating waste requires consideration of the geometry of disposal to control the thermal impact, while non-heat generating wastes can be stored in close proximity if effectively sealed.

Further to the design requirements of the waste material, the host rock for the GDF imposes different design criteria as a result of the thermal, mechanical, hydrogeological, and chemical rock properties. Research has focussed on fractured crystalline rocks [NAGRA, 2009, POSIVA, 2010], fractured volcanic rocks [Birkholzer and Tsang, 2000], low permeability sediments e.g. claystones [ANDRA, 2005, NAGRA, 2009], and salt deposits [Brewitz and Rothfuchs, 2007, Hansen and Leigh, 2011].

Central to the process of radioactive waste disposal is the isolation of the waste from the biosphere. This is typically planned to be achieved through a multi-barrier approach consisting of both engineered barriers (e.g. hydraulic seals), and natural barriers (e.g. the host rock in which the repository is situated) [ANDRA, 2005, Anttila et al., 2008, NAGRA, 2009, POSIVA, 2010, Tweed et al., 2015]. Hydraulic seals form an integral part of the engineered barrier system, both as part of the disposal concept for non-heat generating wastes, and to seal boreholes, galleries and access shafts during the post closure phase. The primary role of the seal is to limit and delay the potential transport of radionuclides from the waste packages to the biosphere by swelling to fill voids and inhibiting advective flow. In research and development programs for radioactive waste disposal seals are primarily composed of unsaturated compacted blocks of bentonite; an expansive clay containing the smectite mineral montmorillonite. Therefore, understanding the behaviour of bentonite and bentonite-sand mixtures during the sealing process is important for safety case and license applications where a certain degree of safety must be demonstrated.

1.1.2 DECOVALEX-2015 and the SEALEX experiments

As the engineering lifetime of a deep geological disposal facility can be in excess of 1,000,000 years, the safety of the multi-barrier system needs to be demonstrated through a combination of experimental work and predictive modelling. In response to the identification of the necessity of robust numerical modelling of technical issues related to the safe disposal of radioactive wastes, the international collaboration DECOVALEX was established in 1992 [Tsang, 2008]. Initiated by the then Swedish Nuclear Power Inspectorate (SKI) (now the Swedish Radiation Safety Authority (SSM)), nuclear waste organisations from around the world were invited to collaborate on the topic of modelling coupled processes relevant to the disposal process [Tsang, 2008]. It was identified that the main processes acting within a disposal system i.e. rock mechanical deformation (M), groundwater flow (H), chemical reactive transport (C), and thermal loading (T), were in-fact coupled, and that this interaction between processes must be considered in numerical modelling of the system. The DECOVALEX project (which stands for the **DE**velopment of **CO**upled process models and their **VAL**idation against **EX**periment) has 5 main objectives relating to these coupled processes [Tsang, 2008]:

- support development of numerical simulators for THM and THMC processes.
- investigate and implement suitable algorithms for THM and THMC modelling
- to compare model calculations to field and laboratory results
- to design new experiments to support code and model development, and
- to study the application of THM and THMC modelling to performance and safety assessment of nuclear waste repositories [Tsang, 2008].

The DECOVALEX project is now into the 6th phase of three year cycles with this project contributing to the most recent phase- DECOVALEX-2015. In DECOVALEX-2015 specific attention has been focussed on the prediction of the hydraulic seal behaviour with Task A investigating the hydro-mechanical saturation behaviour of heavily compacted MX-80 bentonite-sand mixtures [Barnichon et al., 2012]. As with all DECOVALEX tasks, experimental pro-

grammes provide data for model validation and in the case of Task A, the SEALEX experiments at Tournemire, France, fulfill this purpose.

The SEALEX experiments aim to investigate the sealing capacity of different configurations of MX-80 bentonite within the French disposal concept in an argillite host rock [Barnichon et al., 2012]. The experiments consist of a series of steps, which aid model development, from the laboratory scale to full-scale *in situ* tests at the Tournemire Underground Rock Laboratory [Barnichon et al., 2012]. The hydromechanical properties of the bentonite seals are investigated under isothermal conditions with data provided for the following modelling steps:

- Step 0. Laboratory scale hydraulic and mechanical tests used to constrain material parameters for use in later modelling. These include an infiltration test, water retention test, and consolidation tests at varying induced suction pressures.
- Step 1. A 1-10 scale mock-up test of the *in situ* field tests including a uniform technological void and phases of confinement loss.
- Step 2. Hydro-mechanical modelling of the host rock
- Step 3. Modelling of a full-scale *in situ* test with non-symmetric technological void

These experiments are discussed in more detail in Chapters 5, 6, and 7. As this study is focussed primarily on the development of a new hydro-mechanical model for bentonite the work presented herein focusses on steps 0, 1, and 3. To avoid confusion these are renumbered as Step 1, Step 2, and Step 3 respectively for the following work.

1.1.3 Modelling bentonite

The thermal-hydro-mechanical behaviour of bentonite has been the subject of much study over the recent decades through both experiment and numerical modelling e.g. [Dueck et al., 2014, Gaus et al., 2014, Gens et al., 2011, Gens and Alonso, 1992, Low, 1980, Mayor et al., 2014, Pusch et al., 1990, Sellin et al., 2014]. Large international projects comprising both experimental and complimentary modelling work, such as the Full-scale Engineered Barriers Experiment (FEBEX) and Long term Performance of Engineered Barriers (PEBS), have produced significant bodies of research and improved understanding of the coupled behaviour of bentonite [Alonso et al., 2005, Gaus et al., 2014, Mayor et al., 2014, Palacios et al., 2014, Sellin et al., 2014].

A hydraulic seal commonly consists of compacted unsaturated bentonite blocks which expand to fill voids and exert a pressure on the excavation drift during the process of hydration. Modelling developments for bentonite have typically been derived from constitutive modelling of unsaturated soils e.g. [Alonso et al., 1990, 1999, Fredlund and Morgenstern, 1977, Fredlund and Rahardjo, 1993, Gens and Alonso, 1992, Navarro et al., 2014, Sánchez et al., 2005]. These constitutive models couple the hydraulic process to the mechanical process to produce a coupled model that describes the overall soil behaviour. Most models utilise unsaturated Darcy flow to describe the hydraulic process and are therefore commonly defined by the different mechanical models employed.

Elastic and non-linear elastic constitutive models relating the volume, stress state, and hydration state (suction) were developed from the 1960's and broadly fall under the category of a state surface approach [Matyas and Radhakrishna, 1968]. Fredlund and Morgenstern [1977] identified that two independent state variables are all that are required to define the

soil behaviour with this approach. The stress state variable of net mean stress was extended to effective stress by Bolzon and Schrefler [1995]. Analytical expressions for the state surface of bentonite derived from experimental results were determined by Lloret and Alonso [1985] and applied in a coupled thermal-hydrogeological-mechanical model of bentonite by Nguyen et al. [2005]. However, the approach was considered to be limited by a lack of flexibility when considering different stress path behaviour and, due to the elastic assumption, not suitable for modelling unrecoverable strains [Rutqvist et al., 2005, Zhang and Lytton, 2007].

The state surface approach was superseded by the elasto-plastic framework developed by Alonso et al. [1990], which incorporated plastic deformation into the constitutive relationship. These elasto-plastic models were continually developed for both non-expansive and expansive soils e.g. Gens and Alonso [1992] developed a general framework for an elasto-plastic constitutive model, known as the Barcelona Basic Model (BBM), which was subsequently developed for expansive clays by Alonso et al. [1999], Sánchez et al. [2005], and Asensio [2013] (the Barcelona Expansive Model (BExM)), and implemented in different modelling codes [Navarro et al., 2014, Rutqvist et al., 2011]. Alternative frameworks for elasto-plastic models were also developed e.g. Wheeler and Sivakumar [1995], using different stress state variables. Though the state surface approach initially only considered the soil mechanical behaviour to be elastic Zhang and Lytton [2007] show that the elasto-plastic framework developed by Alonso et al. [1990] is based on a specific type of state surface that incorporates unrecoverable strains.

The hydraulic process model has also seen developments for application to expansive clays such as bentonite, with a number of permeability models developed e.g. Achari et al. [1999], Karnland et al. [2006], Komine [2010], Liu [2010], Liu et al. [2011], Pusch and Yong [2003]. The relationship between degree of saturation and total soil suction has been identified as a fundamental parameter for the modelling of unsaturated soils [Fredlund and Xing, 1994] and is typically addressed via two main methods. Standard theories such as the Brookes and Corey function [Brooks and Corey, 1964] and van Genuchten function [van Genuchten, 1980] developed for constant volume conditions have been extended to expansive soils by the incorporation of the sample volume or void ratio e.g. Gallipoli et al. [2003] and Zhou et al. [2012], whereas Dueck [2004] and Dueck and Börgesson [2007] present a stress dependent water retention curve derived from the free swelling water retention properties of bentonite and the confining stress. Furthermore, due to the observed bi-modal pore-size distribution of bentonite [Lloret et al., 2003, Wang, 2012], efforts have been made to include two separate water retention models for the two dominant pore sizes e.g. Alonso et al. [2011], Navarro et al. [2015].

However, there is a trend of increasing complexity in model development as more complex processes and interactions are incorporated. This inevitably results in increasing the number of parameters used to describe the soil behaviour e.g. the BBM requires 14 parameters to describe the mechanical behaviour of a constant volume swelling pressure test [Navarro et al., 2015]. The greater number of parameters provides increasing flexibility to fit data but can also increase the number of potential unknowns and fitting parameters that cannot be verified by experiment.

1.2 Thesis aims and objectives

The overall aim of this study is to develop a comparatively simple hydro-mechanical coupled model based on strain dependent non-linear elasticity for the simulation of the hydration

behaviour of bentonite-sand mixtures tested for hydraulic seals. The main motivation is to model the complex material behaviour with as few parameters as possible. Within this, I aim to extend the current capabilities of OpenGeoSys for bentonite modelling by implementing a number of developments, including:

- develop and implement a strain-dependent non-linear elastic mechanical model that accounts for the development of unrecoverable strains,
- investigate and develop the coupling mechanisms between the hydraulic and mechanical processes as implemented within the open source finite element code OpenGeoSys,
- implement the Dueck method of determining the water retention behaviour, and
- implement a moving finite element mesh to track swelling behaviour and inform the material non-linearity within the mechanical properties.

Finally, I apply the developed model to the results of the SEALEX experiments from the laboratory scale to the full scale *in situ* performance tests.

1.3 Project overview

This project aims to develop a model capable of reproducing the experimental data from the SEALEX experiments with a simple constitutive model. The open source code OpenGeoSys is used and developed to achieve this aim with a specific bentonite model developed and implemented.

In this thesis the hydro-mechanical behaviour of bentonite and the models used to predict behaviour are reviewed and discussed in Chapter 2 and Chapter 3. The development and implementation of the mathematical model (including the implementation of a moving mesh) is presented in Chapter 4. The model is then applied to the three stages of the SEALEX experiments specific to bentonite behaviour in Chapters 5, 6, and 7. The final conclusions are presented in Chapter 8.

The work presented in this thesis has been submitted to a special issue of Environmental Earth Sciences in the following papers:

Fraser Harris A. P., McDermott C.I., Bond A.E., Thatcher K. E., Norris S. (To be Submitted) Non-linear elastic approach to modelling the hydro-mechanical behaviour of the SEALEX experiments on compacted MX-80 bentonite. *Environmental Earth Sciences*

Millard A., Mokni N., Barnichon J.D., Thatcher K.E., Bond A.E., **Fraser Harris A. P.**, McDermott C.I., Blaheta R., Michalec Z., Hasal M., Nguyen T.S., Fedors R., Yi H., Kolditz O. (To be Submitted) Comparative modelling of laboratory experiments for the hydro-mechanical behaviour of a compacted bentonite-sand mixture. *Environmental Earth Sciences*

Millard A., Mokni N., Barnichon J.D., Thatcher K.E., Bond A.E., **Fraser Harris A. P.**, McDermott C.I., Blaheta R., Michalec Z., Hasal M., Nguyen T.S., Fedors R., Yi H., Kolditz O. (To be Submitted) Comparative modelling approaches of hydro-mechanical processes in sealing experiments at the Tournemire URL. *Environmental Earth Sciences*

Much of this work has also been presented in the following peer reviewed iterim project reports:

Bond, A., Thatcher, K., Chittenden, N., McDermott, C., and **Fraser-Harris, A.** (2014a). RWM Coupled Processes Project: First Annual Report for RWM participation in DECOVALEX-2015 Tasks A and C1. AMEC report 18040-TR-002 v2.1.

Bond, A., Thatcher, K., Chittenden, N., McDermott, C. and **Fraser-Harris, A.** (2015a). RWM Coupled Processes Project: Second Annual Report for RWM participation in DECOVALEX-2015 Tasks A and C1. AMEC report 18040-TR-003 v3.0.

Bond, A., Thatcher, K., Chittenden, N., McDermott, C. and **Fraser-Harris, A.** (2015b). RWM Coupled Processes Project: Third Annual Report for RWM participation in DECOVALEX-2015 Tasks A and C1. AMEC Foster Wheeler report 18040-TR-004 v2.0.

Bond, A., Thatcher, K., Chittenden, N., McDermott, C., **Fraser-Harris, A** and Wilson J. (2015c). Final Report of the Coupled Processes Project: Outcomes from DECOVALEX-2015. AMEC Foster Wheeler report 18040-TR-005 v2.0.

Chapter 2

Hydro-mechanical behaviour of bentonite

Bentonite is a naturally occurring clay formed from the weathering of volcanic ash deposits [Deer et al., 1992]. It is principally composed of a swelling smectite clay mineral called montmorillonite but commonly also contains other minor minerals such as quartz, micas, calcite, anhydrite, gypsum, cristobalite, and feldspars, depending on the bentonite origin and stratigraphic location of the deposit [Jönsson et al., 2009, Tang and Cui, 2010]. Commercial bentonites are produced for a wide range of industrial applications, both inside and outside the field of geosciences, due to a range of useful properties. Within geosciences alone, bentonites are used in waste water remediation, as drilling muds in the oil and gas industry, as annular seals for boreholes, as landfill and waste liners, and as hydraulic seals or buffer material for radioactive waste disposal. The main properties that lend bentonites to these applications are their thixotropic properties, ability to take up water and swell to large strains, sorp chemical species to mineral surfaces, and low intrinsic permeability. For the application in radioactive waste disposal the up-take of water, subsequent swelling capacity, and low permeability are the main desirable properties of bentonite that have led to its investigation as a hydraulic seal and buffer material in the engineered barrier system [Wen, 2008]. This chapter outlines the mineralogy and structure of bentonite and the resulting hydro-mechanical behaviour relevant to its use as a hydraulic seal in disposal concepts.

2.1 Bentonite mineralogy and structure

Bentonite is a rock name and therefore represents a clay that is composed of a number of different minerals. The main constituent of bentonite is a sheet silicate known as montmorillonite, which is part of the smectite group. Smectite minerals share the ability to incorporate water and organic materials into their crystal structure leading to structural and volumetric changes [Deer et al., 1992]. Montmorillonite is the most common smectite found in commercial bentonites and is the predominant mineral controlling their hydro-mechanical behaviour. At the individual crystal scale, montmorillonite is a di-octahedral 2:1 smectite comprising a sheet of $\text{Al}_2(\text{OH})_6$ between two sheets of silicate tetrahedra. The sheets are bound together by the sharing of the apical oxygen from the silicate tetrahedra with two out of three OH^-

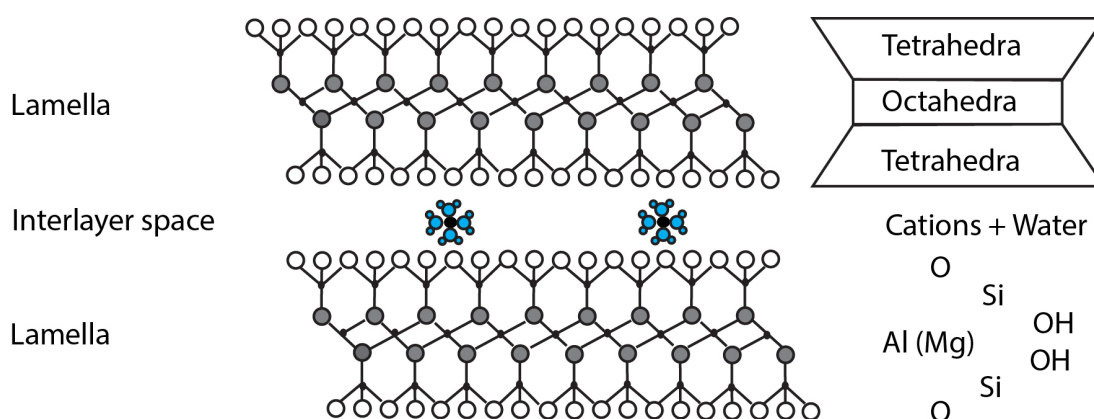


Figure 2.1: A schematic diagram representing the 2:1 arrangement of montmorillonite sheets and the interlamella (interlayer) porosity, (after[Kröhn, 2003])

ions in the aluminium octahedra (Figure 2.1) [Deer et al., 1992]. This structure is similar to other sheet silicates such as pyrophyllite, but the key difference for montmorillonite is the isomorphic substitution of Mg^{2+} for Al^{3+} in the octahedral layer [Low, 1987]. This results in the crystal lattice having a permanent negative charge, which, for sodium montmorillonite, is distributed diffusely over all the surface oxygen atoms [MacEwan and Wilson, 1980]. This charge is balanced by the adsorption of counterions to the surface of the montmorillonite sheet when the montmorillonite is in a dehydrated, or partially hydrated state, and as a result the diffuse negative charge becomes localised at the location of the counterion [Deer et al., 1992, Low, 1987, MacEwan and Wilson, 1980].

Each dehydrated montmorillonite 2:1 sheet does not form a montmorillonite grain in its own right. A mineral grain is composed of a number of sheets arranged in stacks depending on the interlayer cation charge and size [Marcial et al., 2002]. In radioactive waste disposal, montmorillonites that have been under the most scrutiny for practical use are those in which the counterions are either Ca^{2+} or Na^{+} [Cui et al., 2002, Pusch et al., 1990, Ye et al., 2009]. The greater strength of attractive forces between layers in Ca^{2+} montmorillonites results in larger numbers of sheets in each stack e.g. >20-50 as opposed to c.5-10 in Na^{+} montmorillonites [Likos and Lu, 2006, Marcial et al., 2002, Pusch et al., 1990]. The different counterions produce different macrostructural behaviours indicating that the chemical make-up of the mineral is an important control over the behaviour [Marcial et al., 2002]. Some of the differences in behaviour between Ca^{2+} or Na^{+} bentonites have been attributed to the number of stacks that make up a montmorillonite grain [Likos and Lu, 2006, Pusch et al., 1990, Wayllace, 2008]. However, the focus of the experimental study that this modelling study is developed in line with, is the commercial sodium bentonite known as MX-80 (MX-80 is the quality symbol of the production company), and therefore the different behaviours between the two main montmorillonite counterions are not discussed here.

The structure of the montmorillonite sheets and particles, along with accessory minerals, leads to a number of scales of porosity within bentonite:

- Interlamellar or interlayer porosity. The presence of the counterions on the surface of each sheet within a stack results in a layer of micro-porosity on the nanometre scale. This can be exploited by polar liquids, such as water, that hydrate the cations adsorbed

to the surface [Olejnik et al., 1974].

- Intra-particle or Intra-aggregate porosity. Stacks of montmorillonite sheets/particles are arranged into aggregates due to the electrostatic forces acting between charged particles. This leads to a further level of porosity within a single clay aggregate when particles are not perfectly aligned [Agus, 2005, Bradbury and Baeyens, 2003].
- Macro-porosity or inter-aggregate porosity. Equivalent to the porosity that may be characterised in porous media such as sandstones, macro-porosity is pore space that exists between clay aggregates and other accessory minerals [Agus et al., 2010, Gens and Alonso, 1992, Lloret et al., 2003, Marcial et al., 2002, Pusch, 1999, Ye et al., 2009, Yong, 1999a,b].

Agus et al. [2010] suggest a conceptual model of the structural scales of porosity within bentonite (Figure 2.2). This conceptual model corresponds to the pore size distribution data obtained in MIP tests.

Mercury Intrusion Porosimetry (MIP) experiments have been extensively used to identify and characterise the pore size distribution within compacted bentonites and have commonly identified a bimodal distribution in pore throat sizes [Ferrari and Seiphoori, 2015, Lloret et al., 2003, Wang, 2012, Wang et al., 2014, Ye et al., 2009]. In the majority of experiments calculation of the cumulative void volume and the macro-scale calculated void ratio leads to the identification of a significant volume of pores that the mercury was unable to enter with pore throat diameters less than 6 nm [Lloret et al., 2003, Wang et al., 2014]. This nano-scale volume typically corresponds to the interlamellar porosity and, combined with the micro-scale porosity between montmorillonite stacks, forms the intra-aggregate pore volume. Comparison of the derivative of intruded pore volume for samples compacted to different dry densities indicates that the pore volume within grains (interlayer and intra-aggregate porosity) is largely unaffected by the compaction process but the inter-aggregate pore volume is reduced (Figure 2.3) [Lloret et al., 2003]. In this process compressive strains are accommodated by the loss of macro-scale porosity rather than deformation of the aggregates and accessory minerals themselves. The definition of the micro and macro-scale porosity has given rise to the ‘double- structure’ porosity concept for bentonite [Lloret et al., 2003].

2.2 Hydro-mechanical behaviour

Understanding the mineralogy and the structure of montmorillonite within bentonite is important for the development of conceptual models of macro-scale behaviour because processes occurring on the finest structural scale have a significant impact on the bulk behaviour [Likos and Lu, 2006, Wayllace, 2008]. However, the application of bentonite within a radioactive waste disposal facility requires predictions on a scale many orders of magnitude greater than the individual montmorillonite sheets or clay clusters and so understanding the processes occurring at all scales and their contribution to the macro-scale behaviour is vital. Hydrating bentonite is an example of an extremely strongly coupled hydro-mechanical system due to the direct link between the hydration state/water content, sample volume, and mechanical stress. This is due to the capacity of bentonite to swell if unconstrained and/or generate a swelling pressure if hydrated under constant volume conditions [Madsen and Müller-Vonmoos, 1989,

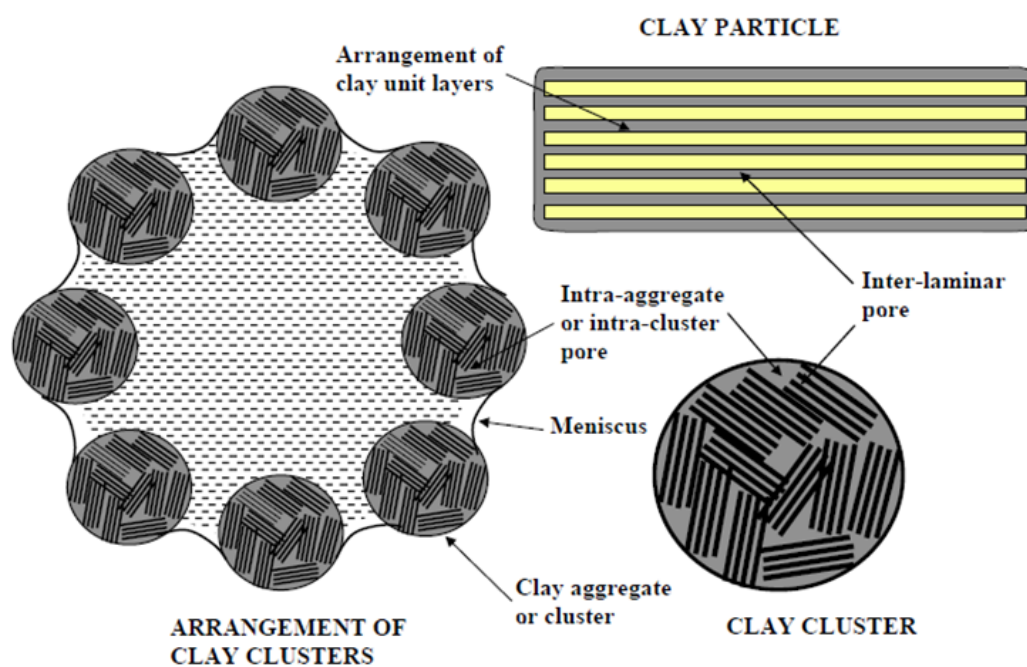
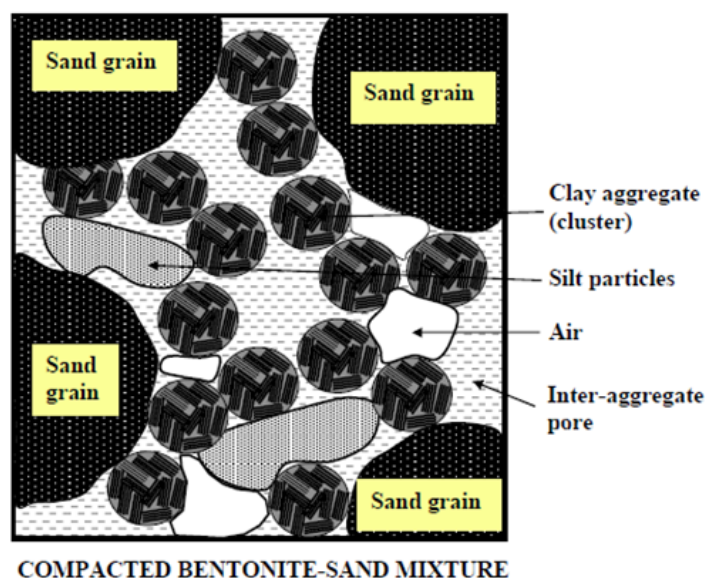


Figure 2.2: Conceptual diagrams of the different scales of porosity within a bentonite sample [Agus et al., 2010]. The finest scale is within a clay particle between individual sheets of montmorillonite. These sheets are arranged into particles that form clusters due to electrostatic forces. Within these clusters an intra-aggregate pore volume exists. These clusters are then arranged within the bentonite as a whole and pore space between clay clusters and other minerals is termed the macro-porosity.

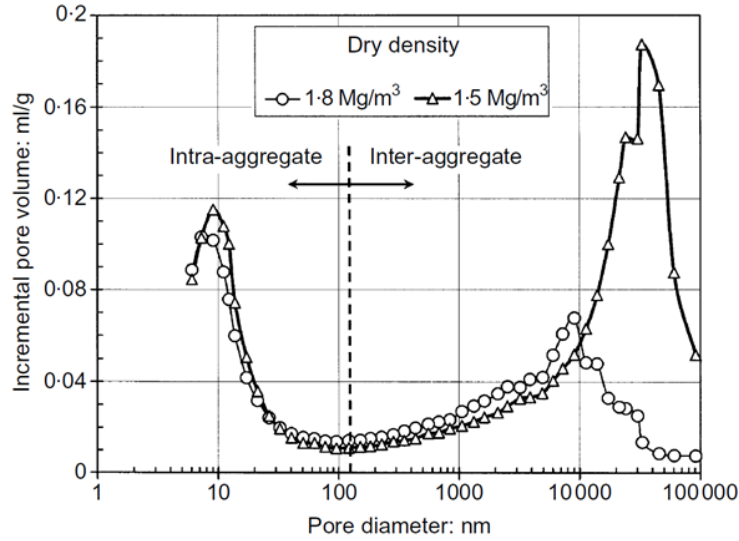


Figure 2.3: Results from Mercury Intrusion Porosimetry tests showing the differential pore throat size distribution of MX80 bentonite [Lloret et al., 2003]

Norrish, 1954]. The fundamental processes controlling this bulk behaviour are introduced here to inform the overall conceptual model.

2.2.1 Concept of Suction

Soil suction is considered to be one of the most important variables when describing the behaviour of unsaturated soils [Fredlund et al., 2012] and, when combined with the water content of the soil, defines the water retention properties. The concept of suction was developed in the early 1900s and later quantitatively defined in terms of thermodynamics by a review panel at the 1965 soil mechanics symposium “Moisture Equilibria and Moisture Changes in Soils” [Fredlund et al., 2012]. Total suction is the total free energy of the water in the soil and can be related to the partial pressure of the pore-water vapour through the following equation [Fredlund et al., 2012]:

$$s = -\frac{RT_K}{v_{w0}\omega_v} \ln\left(\frac{\bar{u}_v}{\bar{u}_{v0}}\right) \quad (2.1)$$

where s is the total suction (Pa), R is the universal gas constant (8.31432 J/(mol K)), T_K is the absolute temperature (K), v_{w0} is the specific volume of water (m³/kg), ω_v is the molecular mass of water vapour (18.016 kg/kmol), $\bar{u}_v$ is the partial pressure of pore-water vapour (kPa), and $\bar{u}_{v0}$ is the saturation pressure of water vapour over a flat surface of pure water at the given temperature (kPa). $(\frac{\bar{u}_v}{\bar{u}_{v0}})$ is the relative vapour pressure or relative humidity (RH (%)).

Total suction at a given temperature is therefore defined in terms of the relative humidity immediately adjacent to the soil water [Fredlund et al., 2012] and comprises two main components:

- **Osmotic suction** is defined as the partial pressure of water vapour in equilibrium with a free solution of soil water relative to that of water vapour in equilibrium with pure water i.e. this is the suction that is caused by the presence of dissolved salts and impurities in

the pore fluid [Agus, 2005, Fredlund et al., 2012].

- **Matric suction** is defined as the partial pressure of water vapour in equilibrium with the pore fluid relative to the partial pressure of water vapour in equilibrium with a solution of the same composition as the pore fluid i.e. this is the suction caused by the soil structure and the location of the pore fluid within the structure [Agus, 2005, Fredlund et al., 2012].

In many non-expansive soils an osmotic suction is induced from the presence of salts within the pore fluid i.e. a sample subjected to a salt solution with a specific relative humidity will have an induced osmotic suction. This suction will cause water of lower concentration to be up-taken into the sample in order to equilibrate the osmotic potential.

As matric suction is a property of the soil brought about by the existence of fluid in partially saturated pore spaces it is commonly associated with the capillary effect. In simple terms the pore network of a soil can be conceptualised as series of tubes of varying radii. As water is the wetting fluid in an air-water system it preferentially exists in contact with the grains of the soil. Due to the surface tension of water a meniscus may form between water held against adjacent grains [Craig, 2004, Fredlund et al., 2012, Helmig, 1997]. The partial pressure of the water vapour above the curved surface is less than that of the reference case (a flat surface) and therefore causes a reduction in relative humidity [Fredlund et al., 2012]. The smaller the radius of the meniscus (i.e. larger curvature), the larger the difference in partial pressure of water vapour immediately adjacent to the soil water and the partial pressure of water vapour above a flat surface of soil water. Consequently a small pore radius results in a large suction that causes water to be drawn up further i.e. the capillary effect. Matric suction (s_m) is therefore often described in terms of the pore water pressure and the pore air pressure and is always less than the air pressure [Fredlund et al., 2012]:

$$s_m = u_a - u_w \quad (2.2)$$

where u_a and u_w are the pore air and pore water pressures respectively. In most unsaturated soils the air pressure is atmospheric pressure and matric suction is negative [Craig, 2004].

Total suction is therefore given by the following equation:

$$s = (u_a - u_w) + \pi \quad (2.3)$$

where π is the osmotic suction [Fredlund et al., 2012].

Yong [1999a] identified that these two components may not be enough to accurately describe the suction behaviour of compacted expansive soils, and instead suggested the use of the term soil potential. Soil potential considers the fact that the matric suction is a combination of both the capillary effect and sorptive processes occurring in clay aggregates and on clay particle surfaces [Yong, 1999a]. This was corroborated by Agus et al. [2010] who investigated the suction properties of bentonite-sand mixtures of different ratios through a variety of experimental methods and compared suction in powdered and compacted specimens. Results showed that total suction is unaffected by void ratio and fabric changes and therefore matric suction in bentonites is predominantly a function of sorptive forces leading to hydration of cations in the montmorillonite structure [Agus et al., 2010].

Soil suction is the main driving force for the saturation process of bentonites and, when combined with the water content data, forms the basis of the hydraulic properties of an unsaturated sample. The experimentally determined relationship between soil suction and water content is termed the water retention curve or soil water characteristic curve (SWCC) and provides the constitutive relationship required to perform numerical simulations on unsaturated soils (as discussed in Chapters 3 and 4).

2.2.2 Stress-state of unsaturated soils

In a saturated soil the concept of effective stress defines the portion of total stress that is accommodated by the mechanical skeleton of the soil i.e. the stress acting on the solid particles of the soil. It is given by:

$$\sigma' = \sigma - u_w \quad (2.4)$$

where σ' is the effective stress, σ is the total stress, and u_w is the pore-water pressure. Effective stress is considered to act in each of the cartesian coordinate axes and, as such, can be described by a stress tensor in which the pore-water pressure is equal in all directions but the total stress may vary. Changes in effective stress in saturated soils are responsible for all measurable phenomenon (distortion, compression, expansion etc.) induced by a change in stress [Fredlund et al., 2012]. The consequence of describing the stress-state with the effective stress principle is that a multi-stress, multi-phase medium can be converted to a mechanically equivalent single stress, single phase medium, which greatly reduces the complexity of determining the stress field [Nuth and Laloui, 2008].

Equation 2.4 shows that the same effective stress can be calculated from a variety of combinations of changes in pore-water pressure and total stress. In saturated soils a change in effective stress caused by either a change in pore-water pressure or total stress has been shown experimentally to result in the same hydro-mechanical response i.e. Terzaghi's effective stress is the 'experimentally true effective stress' for saturated soils [Nuth and Laloui, 2008]. However, for an unsaturated soil an increase in total stress does not necessarily cause the same hydro-mechanical behaviour as the equivalent decrease in pore-water pressure [Fredlund et al., 2012, Nuth and Laloui, 2008]. Therefore, the contribution of total stress and suction must be considered separately in order to extend the effective stress concept to unsaturated soils.

2.2.2.1 Bishop's effective stress

The effective stress of unsaturated soils was first described with a single value effective stress formulation known as the Bishop effective stress:

$$\sigma' = (\sigma - u_a) + \chi(u_a - u_w) \quad (2.5)$$

where σ is the total stress (Pa), u_a is the pore-air pressure (Pa), u_w is the pore-water pressure (Pa), and χ is the Bishop material parameter [Agus, 2005, Fredlund et al., 2012]. The Bishop parameter is a soil parameter that ranges between 0 and 1 that is related to the saturation of the soil [Lewis and Schrefler, 1998]. In fact, in some formulations under the assumption of a microstructurally isotropic material, the Bishop's parameter is replaced with the degree of saturation as they have been shown to be equivalent [Lewis and Schrefler, 1998] Thus the

Bishop's parameter, or saturation, causes a dependency of the effective stress on the hydration state of the sample.

However, as χ is a material parameter and different values of χ can be determined for the same soil when from volume change behaviour and shear behaviour, Fredlund and Morgenstern [1977] suggest that this function is not a description of a stress state but is strictly speaking a constitutive equation.

2.2.2.2 Independent Stress-State variables

To overcome this, the concept of stress-state variables independent of the soil and linked by constitutive relationships were suggested from as early as Biot [1941], developed by Fredlund and Morgenstern [1977], and later widely used in constitutive modelling e.g. Gens and Alonso [1992] and Alonso et al. [1999].

Fredlund and Morgenstern [1977] determined that three possible combinations of stress variables for an unsaturated soil can be determined, but only two independent stress variables are required to represent the unsaturated soil behaviour. These independent stress variable combinations are:

- $\sigma - u_a$ and $u_a - u_w$,
- $\sigma - u_w$ and $u_a - u_w$, and
- $\sigma - u_a$ and $\sigma - u_w$.

The first combination is the most commonly used and refers to the net normal stress and matric suction respectively [Fredlund et al., 2012, Fredlund and Morgenstern, 1977]. Commonly in unsaturated soil applications the pore-air pressure is considered to be constant and equal to atmospheric pressure ($u_a = 0.0Pa$), which simplifies the stress variables to total stress and a negative value of suction [Nuth and Laloui, 2008]. The formulation then requires a double constitutive matrix in a finite element approximation that leads to the separation of the hydraulic and mechanically induced strains.

Nevertheless, many finite element codes were developed for use in saturated fluid flow conditions and the extension of the effective stress concept through the Bishop effective stress provides a useful method to model unsaturated conditions [Nuth and Laloui, 2008]. Furthermore, the single value effective stress concept has been shown to be a suitable stress variable for the modelling of unsaturated soils provided that a second stress variable that corresponds to the work required to change the degree of saturation is included [Gens, 2010, Gens et al., 2006, Houlsby, 1997, Laloui and Nuth, 2005, Nuth and Laloui, 2008]. This ensures the energetic considerations are fulfilled for the work conjugates of the stress and strain variables [Gens et al., 2006, Houlsby, 1997, Laloui and Nuth, 2005, Nuth and Laloui, 2008]. Therefore, the total stress must comprise a mechanical stress component that is responsible for the skeletal strains and a hydraulic stress component that is responsible for the change in saturation [Houlsby, 1997, Laloui and Nuth, 2005]. This can be achieved by suitable choice of constitutive relationships that provide the inter-dependence of effective stress on the hydration state of a soil such as a stress and volume dependent water retention curve function, and the direct influence of a change in suction on the volumetric strain.

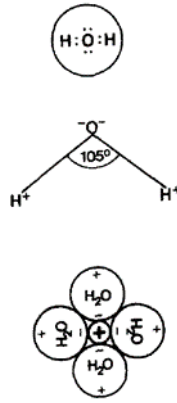


Figure 2.4: Simplified schematic of the polar structure of a water molecule. The molecule is electrically neutral but with uneven charge distribution producing negative and positive dipoles. The negative dipoles are oriented towards the cation thus increasing the ionic radii of the cation and reducing the electrostatic interaction between the particle surface and cation [Madsen and Müller-Vonmoos, 1989]

2.2.3 Swelling

A reduction in effective stress caused by the alleviation of suction / the up-take of water leads to the swelling of montmorillonite particles and aggregates. This is commonly considered to occur via two main mechanisms for the two main sources of suction. Type I, or Crystalline Swelling, is governed by the short scale intra-particle interactions associated with the hydration of interlayer cations that contribute to the matric suction [Agus et al., 2010, Yong, 1999a]. Type II, or Osmotic Swelling, refers to inter-particle repulsive forces caused by the osmotic potential difference between the adsorbed water and the free bulk pore fluid [Laird, 2006, Likos and Lu, 2006, Low, 1987, Norrish, 1954, Wayllace, 2008].

2.2.3.1 Crystalline Swelling

The process of volume expansion by intercalating discrete layers of water molecules between individual montmorillonite sheets is commonly termed crystalline swelling, although it is interchangeable in the literature with Type I swelling [Low, 1980, 1987, MacEwan and Wilson, 1980, Norrish, 1954, Wayllace, 2008]. It is an important process governing the overall system behaviour of bentonite, especially in constant volume conditions and at low water contents [Likos and Lu, 2006]. The structure of water (Figure 2.4) is important in the crystalline swelling process as the charge is unevenly distributed through the molecule. Short range attractive forces produced by hydrogen bonding and/or charged surface-dipole attraction on the negatively charged clay surfaces and partially hydrated cations leads to hydration of the mineral surface and interlayer cation [Wayllace, 2008]. Hydration of the cation is likely to dominate over clay surface hydration and leads to an increase of the ionic radii of the cation and a subsequent swelling of the montmorillonite grain [Wayllace, 2008]. The forces driving this process are termed hydration forces and are typically dominant at low water contents [Wayllace, 2008].

Hydration forces can also be described in terms of relative energy and as such, have also been described as the 'total potential energy of repulsion' [Laird, 2006]. This is a combina-

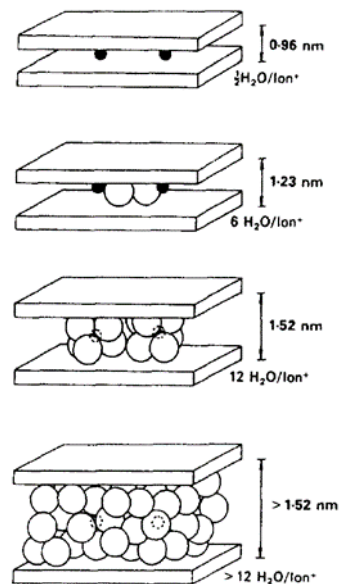


Figure 2.5: Schematic diagrams of crystalline swelling after Madsen and Müller-Vonmoos [1989] showing the uptake of water molecules into the space between montmorillonite sheets. Under constant volume conditions a finite volume of water is able to enter the sample which may result in the number of water mono-layers being restricted during crystalline swelling.

tion of the partial hydration potential energy of the interlayer cations and the negative surface charge sites of the clay [Laird, 2006]. The partial hydration potential energy of the cation refers to the difference in hydration state the cation is currently under and the potential hydration state if the cation was in an equilibrating solution i.e. fully hydrated. Changing the relative humidity alters the potential hydration state but not necessarily the actual hydration state [Laird, 2006]. Changing the potential hydration state of the cation leads to a change in the potential energy of repulsion that can cause volumetric change or indeed, water flow. This concept can also be related to the mechanical influence on a bentonite sample: if the sample is under constant volume conditions the mechanical constraint causes a difference between the actual hydration state and the potential hydration state. In these conditions a finite volume of water may enter the sample because the number of water mono-layers that may develop with crystalline swelling is restricted by the constant volume conditions. This concept is fundamental to the direct coupling method of Dueck suction as discussed in Chapter 3.

Swelling can be measured by the basal spacings derived from X-Ray Diffraction (XRD) [Holmboe et al., 2012, Villar et al., 2012]. A dehydrated sample of montmorillonite has a basal spacing of $c.9.6\text{-}10\text{\AA}$ or $0.96\text{-}1.0\text{nm}$, depending on the interlayer cation type. One mono-layer of water molecules is equal to $c.2.5\text{\AA}$ or 0.25nm . A single layer of hydration leads to a basal spacing of $c.12.2\text{-}12.7\text{\AA}$ and two layers of water correspond to a basal spacing of $c.15.2\text{-}15.7\text{\AA}$ [Holmboe et al., 2012, Villar et al., 2012] (Figure 2.5). Sorption isotherms indicate that hydration of interlayer cations occurs in a step-wise manner corresponding to energy levels of adsorption [Madsen and Müller-Vonmoos, 1989, Sato, 2008].

The structure of the water in the interlayer porosity is not entirely without dispute but it is generally considered to be well structured for sodium montmorillonites, comprising organised layers of water molecules [Madsen and Müller-Vonmoos, 1989, Pusch and Yong, 2006]. The

number of layers of water in the interlayer can reach as many as four for Na^+ montmorillonites (two layers on each sheet), and it is generally accepted that basal spacings increase in a step-wise manner with each water mono-layer [Holmboe et al., 2012, Laird et al., 1995, Pusch et al., 1990, Wayllace, 2008, Yong, 1999a]. The partial hydration state is a useful concept as it explains the step-wise hydration of interlayer cations as observed through experiment [Laird et al., 1995, Likos and Lu, 2006, Sato et al., 1992, Wayllace, 2008]. The configuration of interlayer water is thought to be held against the clay surface in the same manner as a Stern Layer, with the inner Helmholtz plane relating to the first layer of water and the outer Helmholtz plane corresponding to the second layer on each sheet (Figure 2.6).

Yong [1999a] indicates that further from the clay surface the concentration of cations drops off very rapidly, suggesting that the electrostatic forces holding the hydrated cations within the Stern layer have a limited spatial influence. As the maximum number of organised water layers held strongly on the surface of each clay sheet is two, it could be approximated for Na^+ montmorillonites that the Stern layer is on the order of $5\text{\AA}$ or 0.5nm (Figure 2.7). Classical electrical double layer theory indicates that outside this distance a diffuse charged layer exists, which gives rise to the second swelling mechanism. As the dehydrated thickness of a montmorillonite sheet is $c.1\text{nm}$ and the maximum distance over which hydration forces are active is $c.1\text{nm}$, crystalline swelling can account for a doubling in volume of a clay aggregate [Madsen and Müller-Vonmoos, 1989]. It has been shown that the layer charge and location are important factors in the swelling behaviour of montmorillonites [Sato et al., 1992]. Water held in the interlayer is considered to be immobile under normal hydraulic gradients [Pusch and Yong, 2006] and therefore fluid flow occurs within the macro-scale porosity.

The link between overall system volumetric behaviour and crystalline swelling was investigated by Likos and Lu [2006] and Wayllace [2008] for both Na^+ and Ca^{2+} montmorillonites. The sorption isotherms indicating the number of layers of water in the interlayers show that overall volumetric change becomes important once the macroporosity is filled by the swelling clay clusters i.e. swelling is initially accommodated by filling the available macro-pore space. Therefore crystalline swelling is unlikely to result in a doubling of sample volume as suggested by the micro-scale process unless at extremely high dry densities. Hydration forces are dominant for samples under constant volume conditions as swelling is restricted and expansion of the aggregates into the macro-porosity is the only means for swelling to be accommodated before pressure builds on the confining material (the experimental cell or host rock). This in-

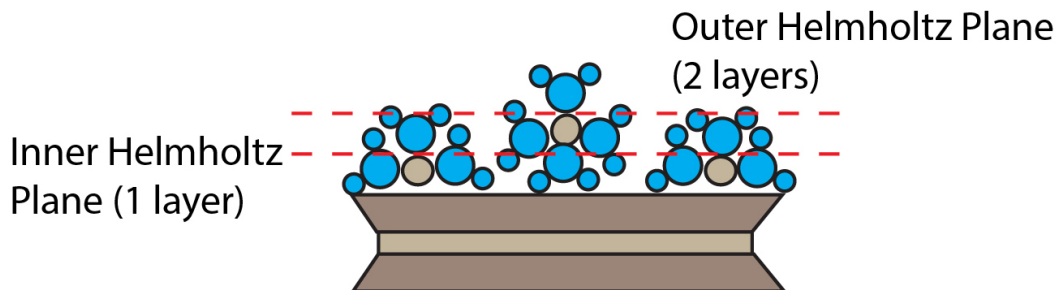


Figure 2.6: A simplified diagram showing the arrangement of water molecules and interlayer cations at the surface of a clay mineral, after Yong [1999a]

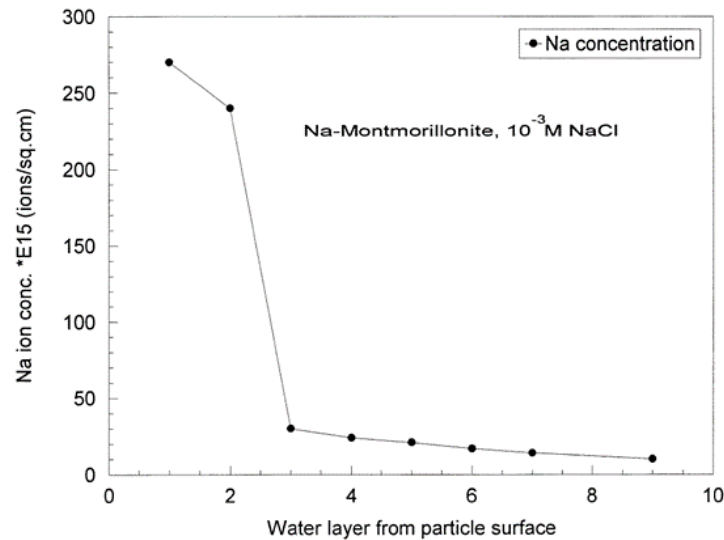


Figure 2.7: Na^+ concentration in water layers with distance from the surface of clay sheets of 2:1 smectite arrangement [Yong, 1999a]

teraction between the micro and macro structural scales results in an added complexity of the hydro-mechanical behaviour.

2.2.3.2 Osmotic Swelling

The hydro-mechanical behaviour of bentonite is further complicated by a second swelling mechanism; osmotic swelling, which, as the name implies, is thought to be driven by an osmotic pressure gradient. This is a different process to that of hydration [Low, 1980] as it is driven by the difference in concentration of ions in the pore water and around the clay surface [Madsen and Müller-Vonmoos, 1989].

This process has been described and modelled using the Diffuse Double Layer theory (DDL) since the 1950's [Norrish, 1954] and has since been developed by many authors e.g. Komine and Ogata [1996, 2003], MacEwan and Wilson [1980], Tripathy et al. [2004], Zhang et al. [1995] and Schanz and Tripathy [2009].

The DDL theory states that the balance of attractive and repulsive forces acting between two parallel plates of montmorillonite controls the distance between the two plates. The forces described by the Gouy-Chapman DDL theory are derived from the electrical potential distribution around the clay

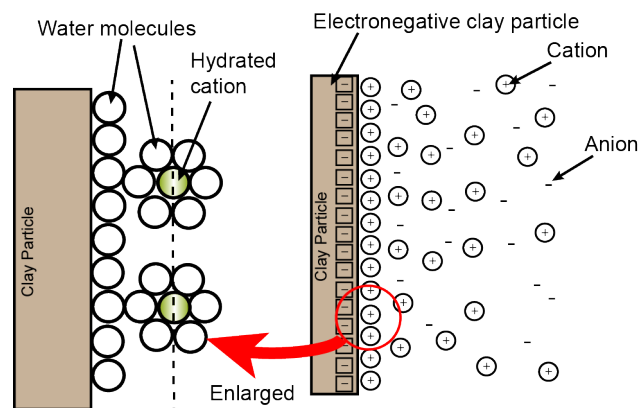


Figure 2.8: Stern Layer configuration of water held against the clay surface with the associated diffuse double layer of charged water [Komine and Ogata, 2003]

layer in the clay-water-electrolyte system [Laird, 2006]. As such, the theory relates the surface charge density, surface potential (as a function of surface charge density), the cation valence, and the electrolyte bulk solution.

The Diffuse Double Layer theory predicts that the electrical potential of the fluid reduces with increasing distance from the clay layer as shown in Figure 2.8. This figure also shows a region on and up to a certain distance from the clay layer where the cation concentration is higher than the surrounding fluid. In this zone the electrical potential falls away in a linear fashion.

This is the Stern Layer and constitutes the region in which the water is bound tightly to the clay surface and cations within the outer Helmholtz Plane. The Stern Layer essentially neutralises some of the surface charge of the clay as the cations are bound to the surface, thereby reducing the chance for impossible electrical potentials to build up [Laird, 2006]. The attractive forces binding the montmorillonite plates together in the DDL theory are described by van der Waals forces as an extension of London's theory for attractive energy between two molecules [Komine and Ogata, 1996]. If the repulsive force overcomes the attractive force then swelling occurs.

It is recognised that this theory for the swelling of bentonite does not hold up well at small basal spacings $\leq 35\text{\AA}$ (high dry densities) and high concentrations of montmorillonite in the bentonite mixture, but is able to explain behaviour up to colloidal bentonite suspensions [Holmboe et al., 2012, Komine and Ogata, 1996, 2003, Laird, 2006, Low, 1987]. The reason for this is that the theory assumes point charges (but in reality the ions are of finite size), and that the process of hydration is different. When ionic concentrations close to the surface are very high i.e. when the montmorillonite concentration is very high and/or the clay is very dense such that interparticle distance is reduced to the same magnitude as interlayer distance, the theory does not predict behaviour accurately [Komine and Ogata, 1996]. Therefore, as this theory is best applied to samples with a basal spacing of over $35\text{\AA}$, it is possible to conclude that the interlayer is likely to be fully saturated before this process begins [Wayllace, 2008].

Osmotic swelling occurs at low suction pressures as shown by the SEALEX water retention curve experiment in Figure 2.9. Furthermore, the Stern Layer configuration shown in Figure 2.8 could be interpreted as the interlayer water bound tightly against the clay surface which has become separated from its opposite partner, or perhaps is on the edge of a pore. The charged water within the diffuse double layer induces an osmotic pressure with respect to the pore water resulting in the ingress of pore water and the further expansion of the clay [Tripathy et al., 2004].

This process is more prevalent in sodium bentonites than calcium bentonites because the Na^+ montmorillonite stacks have fewer sheets and the attractive forces between sheets are smaller [Likos and Lu, 2006]. This allows a larger number of individual sheets to become separated to form electrical double layers through this process, which has become termed 'ex-foliation' [Pusch et al., 1990]. The result for the structure of the bentonite is a homogenisation from peds and aggregates to a honeycomb/bee-hive type structure as shown in Figure 2.10 [Ye et al., 2009]. The explicit modelling of this structure is likely to be extremely challenging in a repository wide context as the structure changes so much on the nano-micro metre scale during exposure to water. Therefore macroscale models often do not explicitly address the fine scale but try to take into account the macroscopic effects of the microstructure behaviour e.g. swelling pressure.

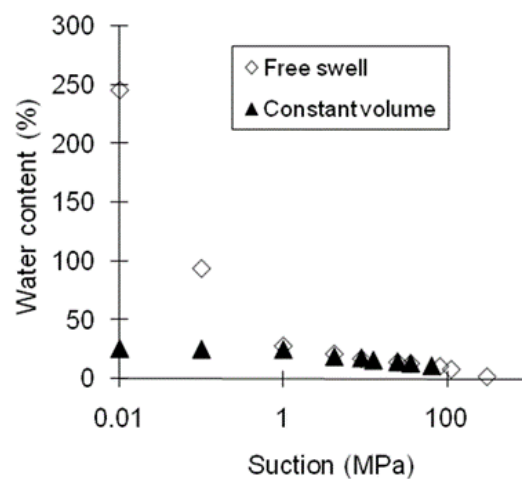


Figure 2.9: Water retention curve results from the SEALEX experiments at Tournamire, France [Wang, 2012]

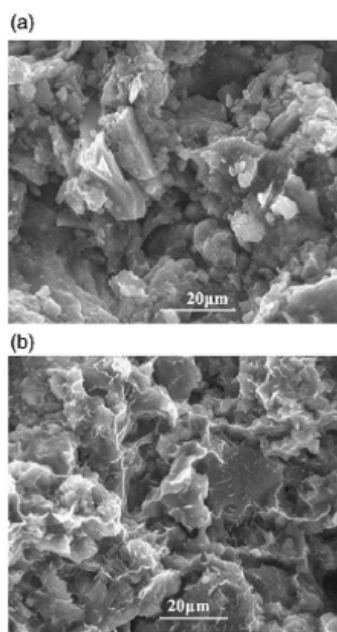


Figure 2.10: An Environmental Scanning Electron Microscope image of compacted bentonite before and after saturation with water. The before image (a) shows a number of aggregates of montmorillonite, but the after image (b) shows a reduction in these aggregates [Ye et al., 2009].

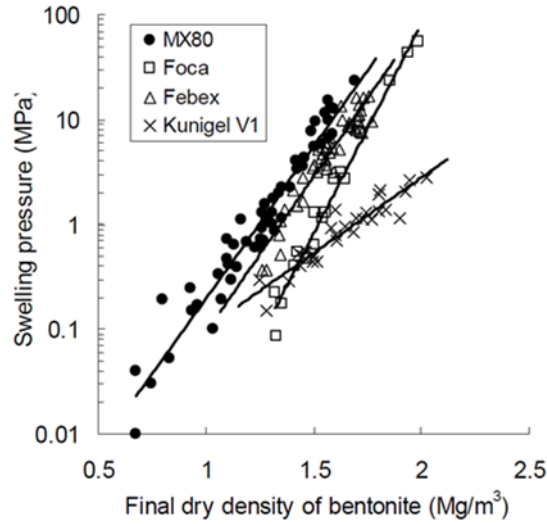


Figure 2.11: A plot of swelling pressure against final bentonite dry density for four different bentonites . The experimental data is fitted with Equation 2.6.

2.2.3.3 Swelling pressure

A key metric in the design criteria of hydraulic seals in radioactive waste disposal is the swelling pressure. Swelling pressure develops as a result of hydration under partial or full confining conditions and is defined as the stress required to maintain constant volume conditions during hydration of a soil from an initially unsaturated state. If the swelling of bentonite is restricted the energy associated with a change in suction is transferred to the constraining material.

As swelling pressure is a key design metric it has been extensively investigated. Through experiment, swelling pressure has been shown to be exponentially related to the dry density of the sample e.g. Komine and Ogata [1996], Pusch et al. [1990] and Wang [2012] among many others. Wang [2012] compared the final dry density of bentonite to the final swelling pressure for different bentonites and determined an empirical relationship that can be parameterised for each bentonite type. Figure 2.11 shows the application of the empirical relationship in Equation 2.6 to four separate bentonites for samples of varying dry density, and highlights the strong link between bentonite dry density and swelling pressure [Wang, 2012].

$$\sigma_s = \alpha_w \times \exp^{\beta_w \rho_d} \quad (2.6)$$

where σ_s is the swelling pressure (Pa), ρ_d is the final dry density of the bentonite, and α_w and β_w are fitting parameters [Wang, 2012].

2.2.4 Consolidation

Consolidation is the process by which volume reduction of a saturated soil takes place as a result of the drainage of water [Craig, 2004] or an applied load. The concept of saturation in an engineering sense is the state achieved when the soil cannot be hydrated further i.e. no more water can enter the sample. During determination of the water retention curve, bentonite in

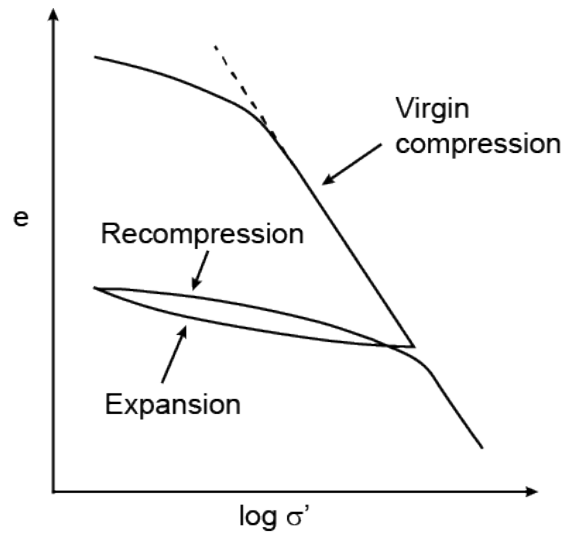


Figure 2.12: A typical plot of void ratio (e) over log net axial stress produced from a one dimensional consolidation test on clay, after Craig [2004]. The hysteresis in expansion and recompression is exaggerated.

a state of equilibrium with a given suction can be considered as a saturated sample for that given suction. This can also be understood by recalling that the micro-structure of bentonite is considered to remain saturated across the range of suction pressures in a similar manner to the way a confined aquifer remains saturated across a range of fluid pressures [Agus, 2005, Alonso et al., 1990, Gens and Alonso, 1992]. In engineering applications the process of consolidation is considered to be the opposite to the increase in volume associated with water uptake i.e. swelling. Consequently, the mechanical behaviour of a soil can be determined from standardised laboratory tests such as the one dimensional oedometer consolidation test [Craig, 2004] as performed in the SEALEX experiments modelled in this study [Wang, 2012]. A soil sample saturated to a given suction value is subjected to a loading path followed by an unloading path and a plot of the void ratio (e) at a given net axial stress is produced e.g. Figure 2.12. Typically this plot is in the form of void ratio over log net axial stress and can be used to interpret specific soil properties.

Two distinct gradients can be determined from these plots with the break in slope providing an indication of the maximum axial stress the soil has previously been subjected to: the pre-consolidation pressure [Craig, 2004]. Upon unloading, an expansion takes place that follows a similar gradient to that of the compression at stresses below the pre-consolidation pressure. Further loading then follows this path again until the new pre-consolidation pressure is exceeded and the soil continues to deform along the same slope as in the previous loading cycle. The steeper slope is termed the virgin consolidation slope as it represents the change in void ratio with stress for a normally consolidated material [Craig, 2004].

The behaviour observed in Figure 2.12 has been interpreted in terms of the mechanical processes of elasticity and plasticity, or both. Elasticity is characterised by recoverable strain behaviour such that a material can be stressed to induce strain, but when that stress is removed the material will return to its original state [Lewis and Schrefler, 1998]. Therefore, the elastic process is independent of the strain history of the material. Plasticity is characterised by non-recoverable strain behaviour and states that a material stressed to a point beyond its yield

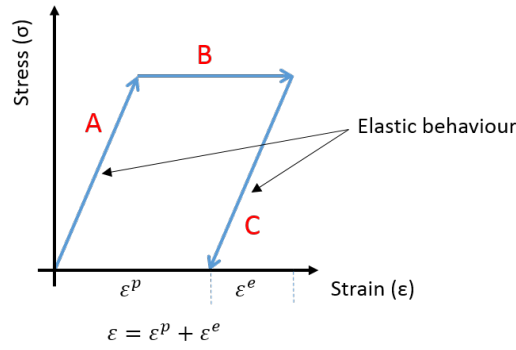


Figure 2.13: A stress-strain diagram showing the concepts of elastic and plastic behaviour for a sample that behaves in an elastic-perfectly plastic manner (modified from Lewis and Schrefler [1998]). In zone A the sample is deforming elastically; removing the stress will result in the sample returning to its initial state. In zone B a yield stress has been exceeded and the sample continues to deform without a corresponding increase in stress. This strain is termed the plastic strain (ϵ^p). In zone C the stress is removed and the sample behaves elastically once more but cannot return to its original state because of the plastic non-recoverable strains that occurred during zone B.

strength will cause permanent deformation of the material and it cannot return to its original state when the stress is removed [Lewis and Schrefler, 1998]. These concepts are graphically represented in Figure 2.13 for a simplified case. A sample under stress conditions corresponding to zone A will return to the origin if the stress is removed but, once the stress exceeds the yield strength, further deformation occurs without a continued build up in stress and when the stress is then removed the sample cannot return to its initial conditions i.e. it has non-recoverable strain. The slope of the elastic behaviour (A and C) defines the elastic material properties of the solid and the gradient of the line B defines the plastic behaviour i.e. strain hardening, strain softening, or the perfect plasticity scenario shown in Figure 2.13.

The behaviour shown in Figure 2.13 is for a simplified case of elastic-perfectly plastic behaviour but in reality the mechanical behaviour of soils exhibits significant non-linearity [Craig, 2004, Lewis and Schrefler, 1998]. Commonly, zone A is not a simple straight line but takes a non-linear form which can be modelled either within the context of variable elasticity or through a double elasticity model which switches between two elastic material models depending on whether a yield criteria has been exceeded [Lewis and Schrefler, 1998]. The soil behaviour shown in Figure 2.12 is interpreted in the context of non-linear elasticity and elasto-plasticity and shown in Figure 2.14.

An elasto-plastic interpretation separates the behaviour of the soil along the virgin consolidation line from the compression and rebound behaviour at stresses lower than the pre-consolidation pressure [Lewis and Schrefler, 1998]. On the other hand, the non-linear elastic interpretation defines an increase in material stiffness based on the concept of strain hardening. Incremental calculations of linear elasticity with a variable elastic modulus enable the non-linear nature of the behaviour to be calculated [Fredlund et al., 2012, Fredlund and Rahardjo, 1993]. At the point of stress unloading non-recoverable strains are achieved in a non-linear elastic approach if rebound occurs with a constant mechanical stiffness i.e. rebound with the new elastic modulus. In the context of the double structure of bentonite the consolidation behaviour can be interpreted as a rearrangement of grains that leads to a destruction of the macro-porosity and leads to permanent void ratio change [Gens and Alonso, 1992, Laird,

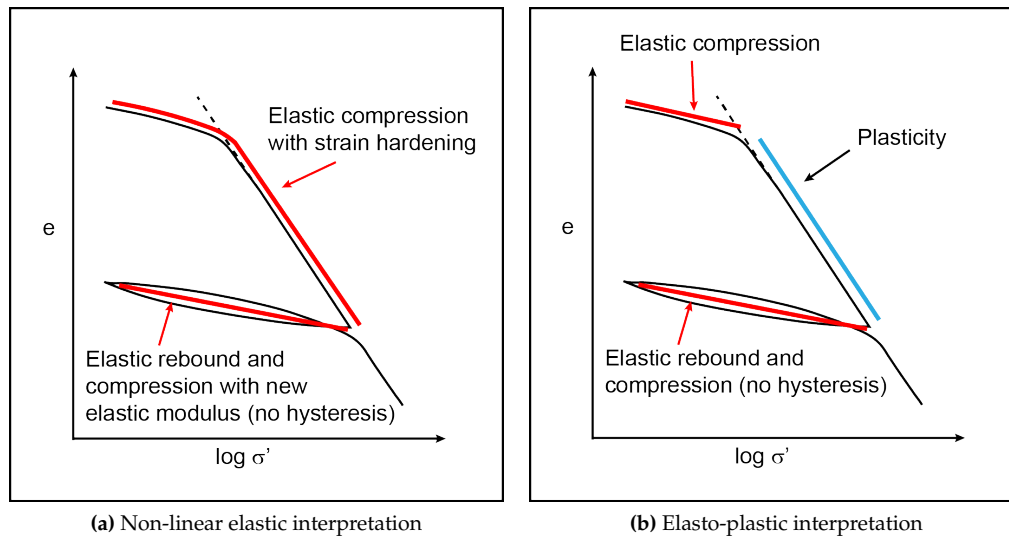


Figure 2.14: A typical consolidation test result interpreted in the context of non-linear elastic strain hardening (a) and elasto-plasticity (b).

2006]. The reduction of macro-void space makes the sample less compressible and therefore represents an increase in material stiffness. Once the macro-void space is consolidated, the expulsion of water from the interlayer space of montmorillonite particles requires increasing amounts of work at lower water contents [Madsen and Müller-Vonmoos, 1989, van Olphen, 1965, Wayllace, 2008], which manifests itself in a further increase in material stiffness.

2.2.4.1 Collapse behaviour

Unsaturated soils and soils of high plasticity can also have the property of wetting induced collapse behaviour [Fredlund et al., 2012, Gens, 2010, Lewis and Schrefler, 1998, Lloret et al., 2003]. Collapse behaviour of this nature has been a driving motivation for the development of elasto-plastic models in unsaturated soil mechanics [Nuth and Laloui, 2008]. A reduction in volume with continued hydration is in apparent contradiction to the single value effective stress concept and is often cited as a validation of the use of the independent stress variables approach over the Bishop's effective stress [Agus, 2005, Fredlund and Morgenstern, 1977, Gens, 2010, Nuth and Laloui, 2008].

This behaviour has been interpreted in a number of ways with respect to bentonites and the double porosity structure. The non-expansive unsaturated soil explanation for wetting induced collapse is as a result of cementing bonds between the grains in initially dry samples being broken by the hydrating water [Nuth and Laloui, 2008]. During the process of hydration this leads to reduction in material stiffness and a potential consolidation under constant loads [Gens, 2010, Nuth and Laloui, 2008]. However, during drying the opposite behaviour is observed and the apparent strength of the material increases with increasing suction leading to the observation of increasing pre-consolidation pressure with increasing suction [Agus, 2005, Nuth and Laloui, 2008]. For bentonite, which possesses a clearly bi-modal pore size distribution and double structure, the collapse mechanism is interpreted as a collapse of the macro-structure in response to the developed swelling pressure/confining load [Lloret et al.,

2003], or by structural rearrangement of clay clusters within the sample as a result of the frictional coefficient of the soil being overcome by wetting-induced shear forces at the micro-scale [Agus, 2005]. These mechanisms consider the wetting-induced plastic collapse phenomenon to be as a result of the interaction between micro-structural processes and the collapse of the macro-structure [Lloret et al., 2003].

Chapter 3

Constitutive Modelling of Bentonite

Constitutive hydro-mechanically coupled numerical models of bentonite have been developed over the past few decades in response to the requirement for predictive models to simulate the behaviour of bentonite under repository conditions [Alonso et al., 1990, 1999, Fredlund and Morgenstern, 1977, Gens and Alonso, 1992, Lloret and Alonso, 1985, Navarro et al., 2015, Pham, 2005, Sánchez et al., 2005, Wheeler and Sivakumar, 1995]. Bentonite represents a specific type of unsaturated soil due to the significant volumetric changes or build up of swelling pressure that can occur as a result of hydration from an initially unsaturated compacted state. Modelling of the hydraulic and mechanical processes requires a constitutive modelling framework that allows the close coupling between the two processes to be accounted for [Gens et al., 2006]. The developed models are considered within the umbrella term of volume-mass constitutive models as they relate the overall sample volume and water content variables to the stress variables [Pham, 2005]. This chapter presents the main features of a number of constitutive modelling approaches used to simulate bentonite behaviour. Typically modelling frameworks have been developed from a mechanical perspective with the constitutive framework developed to include the influence of the hydraulic process. As such, this chapter first addresses the constitutive models from the view point of the chosen mechanical model and then considers the key aspects of hydraulic models.

3.1 Constitutive models

There are a number of constitutive frameworks used to model bentonite which differ mainly upon the choice of mechanical model employed and the description of the stress state. The modelling of the mechanical behaviour can be broadly divided into elastic or elasto-plastic process models as shown in Figure 3.1. Within the elastic framework non-linearity can be incorporated through an incremental calculation method in which the elastic properties are updated for each incremental change in stress [Fredlund et al., 2012, Fredlund and Rahardjo, 1993, Lewis and Schrefler, 1998]. The elasto-plastic models can be further sub-divided into those which consider perfect plasticity and those that incorporate strain hardening and softening. In this section, the elastic approach is first considered with examples, followed by the elasto-plastic strain hardening approach.

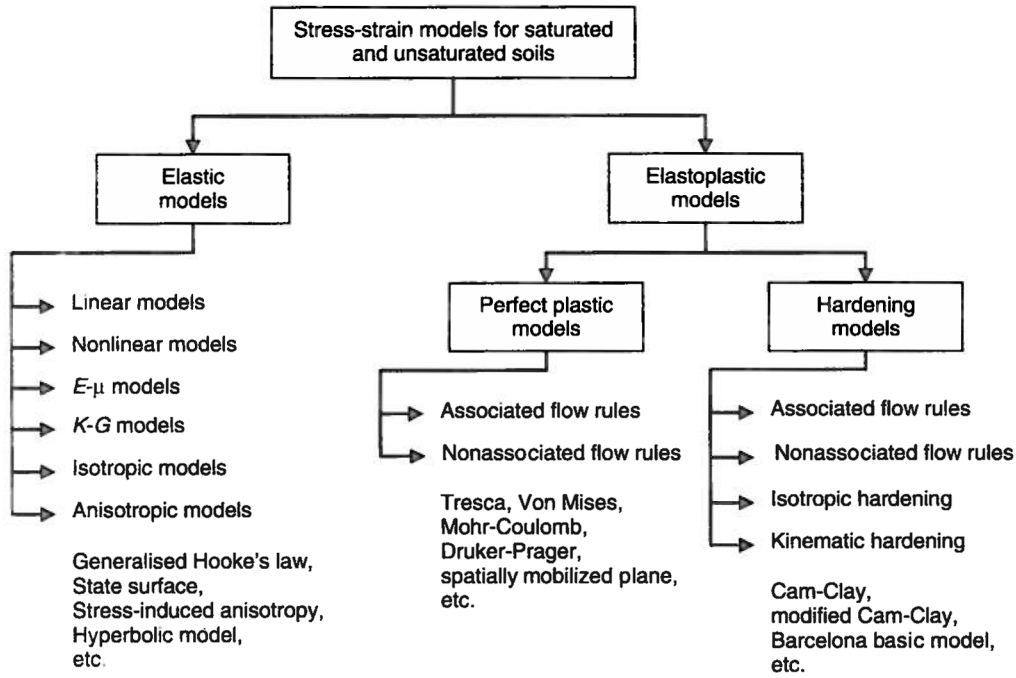


Figure 3.1: A diagram showing the different stress-strain constitutive models employed for the mechanical calculation of unsaturated soil behaviour. These are broadly divided into elasticity based models and elasto-plastic models [Fredlund et al., 2012].

3.1.1 Volume-mass constitutive models

Central to the development of volume-mass constitutive models is the continuity requirement, which states that the change in volume of a sample with incompressible particles is a function of the change in water volume, change in air volume, and the change in the volume of the 'contractile skin' (the so-called fourth phase- the air-water interface) [Fredlund et al., 2012, Fredlund and Rahardjo, 1993, Pham, 2005]. Considering the volume change of the air-water interface to be internal to the soil element allows the term to be neglected from the volume continuity requirement [Pham and Fredlund, 2011], resulting in:

$$\frac{\Delta V_v}{V_0} = \frac{\Delta V_w}{V_0} + \frac{\Delta V_a}{V_0} \quad (3.1)$$

where V_v is the total volume of the voids in the sample (assuming incompressible grains), V_0 is the initial total volume of the soil element, V_w is the water volume, and V_a is the volume of the air [Fredlund et al., 2012, Pham and Fredlund, 2011]. Consequently, the linking of the stress state variables to volumetric variables such as water volume and void ratio, to satisfy the continuity requirement led to the definition of volume-mass constitutive surfaces that were considered to bound the soil behaviour [Fredlund et al., 2012, Fredlund and Rahardjo, 1993, Lloret and Alonso, 1985, Nguyen et al., 2005, Pham, 2005].

These state surfaces can be plotted on a 3D graph as in Figure 3.2 (after Pham and Fredlund [2011] and Fredlund et al. [2012]) and describe the volumetric behaviour of the soil volume (a) and the water volume (b) with respect to changes in the independent stress state variables [Pham, 2005].

However, a constitutive state surface is not unique for an unsaturated soil under varying

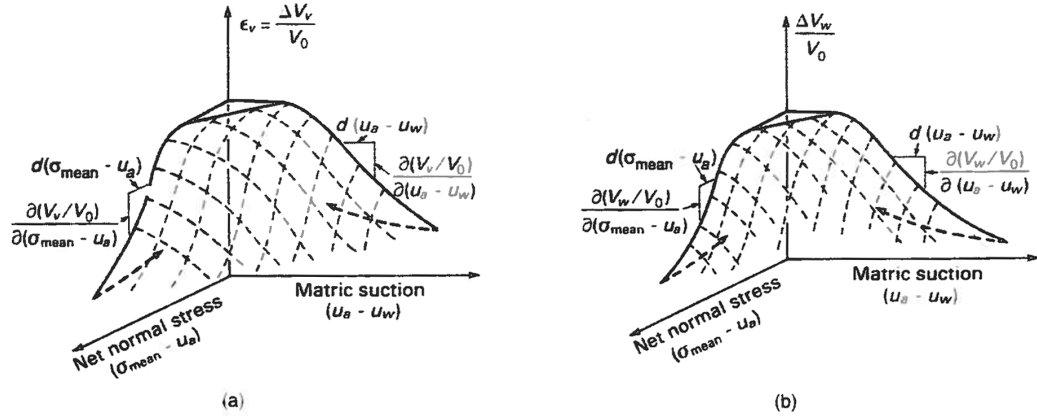


Figure 3.2: Schematic diagrams of the constitutive state surfaces for the void ratio (a) and the water volume (b) with respect to the independent stress variables net mean stress and suction [Fredlund et al., 2012]

stress conditions due to hysteresis effects of loading-unloading cycles and/or wetting-drying cycles [Pham and Fredlund, 2011] i.e. there is no single constitutive state surface that can describe the soil state for all stress paths. For example, hydraulic hysteresis, which results in different soil water contents depending on whether the soil is following a drying or wetting path, is common in unsaturated soils [Fredlund et al., 2012, Gens et al., 2006, Pham and Fredlund, 2011, Rutqvist et al., 2005], and mechanical hysteresis is also observed during loading-unloading cycles [Gens et al., 2006]. Stress path dependency is present for soils which are subjected to a drying process, but a soil that is only subjected to a wetting path exhibits stress path independent behaviour [Pham, 2005].

The subsequent development of elasto-plastic constitutive frameworks during the early 1990's [Alonso et al., 1990, Gens and Alonso, 1992] led to their extensive use in the simulation of unsaturated soils due to their capacity to incorporate observed phenomenon such as hydraulic hysteresis, suction hardening, and wetting induced collapse. Nevertheless, the constitutive surface remains a useful concept within soil mechanics and fundamental for the visualisation of the effects of a change in the soil stress state [Pham, 2005]. Zhang and Lytton [2007] have even shown that the constitutive state surface approach can be used to explain the key concept in one of the most widely used elasto-plastic constitutive frameworks for soil mechanics modelling: the Loading-Collapse curve in the Barcelona Basic Model.

3.1.2 Elasticity based constitutive models

Elastic and non-linear elastic approaches were developed to describe the volume-mass constitutive surfaces of unsaturated soils in the 1970's and 1980's and can be broadly divided into those which are physically based with physical soil parameters, and those that are based on an empirical approach or a surface fitting approach [Pham, 2005].

3.1.2.1 Physically based models

An example of a physically based elastic model describing the volume-mass constitutive surfaces is that of Fredlund and Rahardjo [1993]. In this work, volumetric change was considered

to be a function of the change in porosity of a sample i.e. the grains were incompressible and any strain was accommodated by a change in porosity. Therefore, overall volume change, defined as the volumetric strain, was equivalent to the change in the volume of the voids [Fredlund et al., 2012, Fredlund and Rahardjo, 1993]:

$$\epsilon_v = \frac{\Delta V_v}{V_0} \quad (3.2)$$

An elasticity based model for volumetric strain was proposed in which volumetric strain is calculated from both the mechanical load (net normal stress) and the hydraulic load (suction) in incremental form after Fredlund et al. [2012], Fredlund and Rahardjo [1993]:

$$d\epsilon_v = 3\left(\frac{1-2\mu}{E}\right)d(\sigma_{mean} - u_a) + \frac{3}{H}d(u_a - u_w) \quad (3.3)$$

where E is the elastic modulus of the mechanical soil structure (Pa), μ is Poisson's ratio (-), σ_{mean} is the mean normal stress (Pa) $((\sigma_x + \sigma_y + \sigma_z)/3)$, u_a is the air pressure (Pa) (equal to zero in Richards' approximation), u_w is the water pressure (Pa), and H is the modulus of elasticity for the soil structure with respect to a change in suction (Pa) [Fredlund and Rahardjo, 1993]. At each increment of stress the elastic modulus is updated to produce a non-linear elastic soil behaviour using an elastic assumption. Equation 3.3 is used to determine the sample volume constitutive surface. A similar expression to Equation 3.3 can be written to define the change in water volume:

$$\frac{dV_w}{V_0} = \frac{3}{E_w}d(\sigma_{mean} - u_a) + \frac{d(u_a - u_w)}{H_w} \quad (3.4)$$

where E_w is the 'water volumetric modulus' for a given change in net mean stress, and H_w is the 'water volumetric modulus' for a change in suction [Fredlund et al., 2012, Fredlund and Rahardjo, 1993, Pham, 2005].

The non-linear elastic model of Fredlund and Rahardjo [1993] has since been extended to include both elastic and plastic processes by Pham [2005] and Pham and Fredlund [2011]. This model takes into account the pore size distribution of the soil and identifies collapsible and non-collapsible pores in order to account for plastic collapse of the larger pores during hydration [Pham, 2005, Pham and Fredlund, 2011]. The deformation of the pores results in a change to the pore size distribution, which allows hydraulic hysteresis to be included [Pham, 2005, Pham and Fredlund, 2011]. Furthermore, the yield surface is closely linked to the pore size distribution which provides a strong coupling between the hydraulic and mechanical processes [Pham and Fredlund, 2011]. Although, both plastic and elastic deformations are accounted for the model is not defined as an elasto-plastic model as it does not take into account the individual influences of each principle stress direction [Fredlund et al., 2012]. This model has primarily been applied to non-expansive unsaturated soils.

3.1.2.2 Surface fitting/empirical models

Lloret and Alonso [1985] presented an empirical fit for the soil volume state surface that was subsequently used to model the volumetric behaviour of compacted bentonite by Nguyen et al. [2005]. Void ratio (e (-)) is a function of the soil suction (s (Pa)) and mean net stress ($-\sigma_m''$ (Pa)):

$$e = A + B \ln(-\sigma_m'') + C \ln(s + p_a) + D \ln(-\sigma_m'') \ln(s + p_a) \quad (3.5)$$

where p_a is the atmospheric pressure, and A , B , C , and D are all fitting parameters [Nguyen et al., 2005, Pham, 2005]. The constitutive surface calculated by this equation may not be unique for the soil due to the hysteresis effects but can be effectively applied if only the wetting phase is considered [Pham, 2005]. However, the parameters for both the physically based and empirical models are not directly measurable and involve calibration to experimental data Pham [2005]. A further limitation is their inability to account for the wetting induced collapse phenomenon.

3.1.2.2.1 Cui et al. [2002] non-linear elastic model

An alternative empirical non-linear elastic approach was proposed by Cui et al. [2002] to model behaviour of a Ca^{2+} bentonite observed in the laboratory. Experimental results on heavily compacted bentonites with a dry densities of 1.85 Mg/m^3 suggested that hysteresis in wetting-drying and loading-unloading cycles was not significant. Consequently a non-linear elastic approach was adopted in favour of an elasto-plastic model.

The model was developed from the Olsen and Mesri conceptual models for the mechanical processes and physico-chemical processes [Cui et al., 2002]. Each consists of three variables, two of which are the geometric arrangement of particles and the particle shape (defined by the ratio of diameter to particle thickness). The third parameter of the mechanical model is the coefficient of friction, and the third physico-chemical parameter comprises chemical variables such as surface charge, cation valence, dielectric constant etc. [Cui et al., 2002]. These processes are coupled by their dependency on the density of the material; at low densities the contact angle is high and mechanical processes dominate over physico-chemical. However, as compression occurs, the contact angle decreases and physico-chemical processes become more important [Cui et al., 2002]. Strain hardening is implicit in the conceptual model because the increasing dependency on physico-chemical processes results in a decrease in compressibility i.e. increase in elastic modulus [Cui et al., 2002]. The authors attribute the reversibility of the mechanical behaviour to the increase in dominance of the physico-chemical effects at very high dry densities [Cui et al., 2002].

The basis of the model for volumetric behaviour is a concept termed the Critical Swelling Curve (CSC), which defines a threshold where the volume increase caused by a reduction in suction is balanced by the external load [Cui et al., 2002]. This could also be described as a curve that defines the swelling pressure at different suctions. The CSC is used within the model to define whether volume change is occurring or if the applied load is enough to balance the pressure produced by swelling. A sample at a stress state corresponding to a position above the CSC will swell [Cui et al., 2002]. When the suction reaches a point coinciding with the CSC volumetric change stops and further hydration occurs with no volume change (Figure 3.3). If, however, a sample is subjected to a consolidation test at constant suction then void ratio will decrease dependent on the coefficient of compressibility (itself a function of the suction) until the stress state coincides with the CSC. At this point the CSC acts as a failure criterion and further void ratio change is a function of the virgin consolidation curve (Figure 3.4) [Cui et al., 2002].

Cui et al. [2002] proposed an empirical relationship for the volume change caused by a

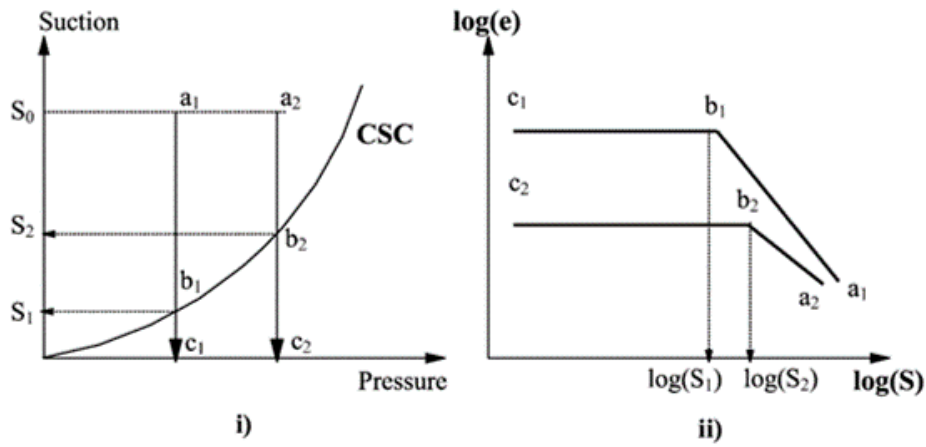


Figure 3.3: Schematic diagrams showing the control of the Critical Swelling Curve during hydration at constant stress. The stress path is shown in (i) and the corresponding volumetric behaviour shown on a $\log(\text{void ratio})$ - $\log(\text{suction})$ plot in (ii).

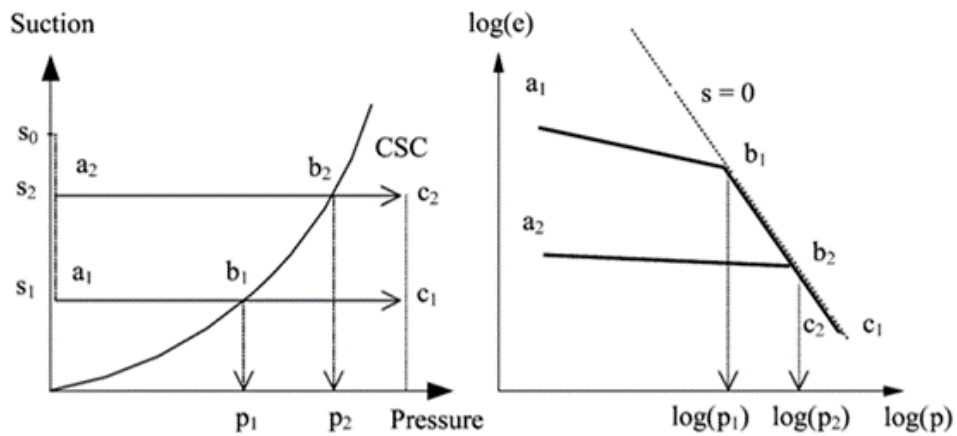


Figure 3.4: Schematic diagrams showing the control of the Critical Swelling Curve during loading at constant suction. The stress path is shown on the left and the corresponding volumetric behaviour shown on a $\log(\text{void ratio})$ - $\log(\text{stress})$ plot on the right.

change in stress (p):

$$e = A_p(s) \left(\frac{p}{p_c} \right)^{N_p(s)} \quad (3.6)$$

and a change in suction:

$$e = A_s(p) \left(\frac{s}{s_c} \right)^{N_s(p)} \quad (3.7)$$

where e is the void ratio, $A_p(s)$ is the value of void ratio when mean stress (p) is equal to a reference stress (p_c), $N_p(s)$ is the slope of the data in a $\log(p):\log(e)$ plot, $A_s(p)$ is the void ratio when suction (s) is equal to a reference suction (s_c), and $N_s(p)$ is the slope of the compression index in a $\log(p):\log(e)$ plot [Cui et al., 2002].

A change in volumetric strain caused by a change in net mean stress at constant suction is calculated from:

$$d\epsilon_v = A_p(s) N_p(s) \frac{1}{1+e} \left(\frac{p}{p_c} \right)^{[N_p(s)-1]} \frac{dp}{p_c} \quad (3.8)$$

The parameters $A_s(p)$, $A_p(s)$, $N_s(p)$, and $N_p(s)$ are determined with four additional fitting parameters.

The CSC is defined from the following equation:

$$\left(\frac{s}{s_c} \right) = \left[\frac{A_p(0) \left(\frac{p}{p_c} \right)^{N_p(0)}}{a \left(\frac{p}{p_c} \right)^d} \right]^{\frac{1}{c \ln \left(\frac{p}{p_c} \right) + b}} \quad (3.9)$$

where a , b , c , and d are fitting parameters used to determine $A_s(p)$, $A_p(s)$, $N_s(p)$, and $N_p(s)$ [Cui et al., 2002]. The lack of requirement to model the plastic behaviour greatly simplifies the model, although the equations derived to define the CSC are an empirical fit and are restricted to reversible volumetric behaviour. Furthermore, the CSC does not pass through the origin and therefore overestimates the swelling pressure at low suctions [Cui et al., 2002].

3.1.3 Elasto-plastic models

Elasto-plasticity, as the name suggests, is the combination of elastic and plastic behaviour. It defines a range of stress conditions in which a sample may deform elastically, limited by stress conditions under which plastic yielding and failure occur. The accumulation of strain is a function of the increase in stress (elastic/non-linear elastic behaviour) until a yield stress is exceeded, after which further strain accumulates without a corresponding increase in stress (plastic behaviour). Processes such as strain hardening (an increase in stress with increasing strain) and strain softening (a decrease in stress with increasing strain) are observed in many materials depending on their material characteristics [Lewis and Schrefler, 1998]. In purely mechanical applications, models developed to predict these processes include the Mohr-Coulomb failure criteria used widely in rock mechanics, and the Cam-Clay model derived from the Critical State Theory of soil mechanics. Both have been used and adapted in the simulation of clay behaviour e.g. Schofield and Wroth [1968] introduce the Cam Clay model, Börgesson et al. [1995] describe an adapted Mohr-Coulomb failure model, and Alonso et al. [1990, 1999], Gens and Alonso [1992] adapt the Cam Clay model to include a dependence of the failure criterion

on suction. The Cam Clay model is briefly explained as a precursor to the Barcelona models that are widely used in soil mechanics.

3.1.3.1 Cam Clay Model

The Cam-Clay models developed out of the Critical State Concept of soil mechanics. This concept, developed by Roscoe, Schofield, and Wroth in the 1950s [Schofield and Wroth, 1968], is the idea that a single surface can be defined that limits all possible stress states of an isotropic clay, and that all the possible effective stress paths converge towards a single line on this surface, known as the critical-state line (CSL) [Lewis and Schrefler, 1998]. The Critical State Line (SS in Figure 3.5) is defined in terms of mean effective stress (p), deviatoric stress (q), and volume (v), and defines the conditions at which a sample can accumulate shear strains without any subsequent changes in p , q , or v [Craig, 2004]. The material behaves as a frictional fluid under these conditions [Lewis and Schrefler, 1998].

The Cam-Clay model is a critical-state model defined in terms of the energy of the system and determines the mechanical response of a specimen to an applied load in terms of the work done during loading and unloading. The stress state is defined in terms of mean pressure (p) and deviatoric stress (q), in which an elastic regime and a yield surface are defined [Borja and Lee, 1990]. Mean pressure is also defined as volumetric stress and is expressed as:

$$p = \frac{1}{3} \text{tr}(\boldsymbol{\sigma}) \quad (3.10)$$

The deviatoric stress is given by:

$$q = \sqrt{\frac{3}{2} \|\boldsymbol{\iota}\|} \quad (3.11)$$

where $\boldsymbol{\iota}$ is:

$$\boldsymbol{\iota} = \boldsymbol{\sigma} - \frac{1}{3} \text{tr}(\boldsymbol{\sigma}) \mathbf{1} \quad (3.12)$$

where $\mathbf{1}$ is the Kronecker delta [Borja and Lee, 1990]. The yield surface is defined by:

$$F = \frac{q^2}{M^2} + p(p - p_{con}) = 0 \quad (3.13)$$

where F is the failure ellipsoid, M is the slope of the critical state line in a $p - q$ plot, and p_{con} is the pre-consolidation pressure [Borja and Lee, 1990].

For normally consolidated samples the curve defining the stress state (NN in Figure 3.5) is also defined in terms of p - q - v space and the surface that joins this and the CSL is known as the state boundary surface for normally consolidated clays [Craig, 2004]. For over consolidated clays, another curve that defines the point at which the minor principle stress is zero (because the clay is assumed to be unable to withstand tensile stresses) is drawn in p - q - v space (TT in Figure 3.5). From the origin to this line, the state surface boundary is defined by a line (V-U) at a slope of 3:1 because $\frac{q}{p'} = 3$ when $\sigma_3 = 0$. The surface between this line, the over consolidated curve, the CSL, and the normal consolidation curve defines the complete state boundary surface for normal and over-consolidated clays as shown in Figure 3.5.

Changes in the stress state are brought about by the application or removal of the external load. Figure 3.6 illustrates the concept of the Cam Clay model in the context of a one-dimensional consolidation test [Schofield and Wroth, 1968]. Under isotropic loads the Cam-clay exhibits an elastic response to an applied load until the yield stress (pre-consolidation

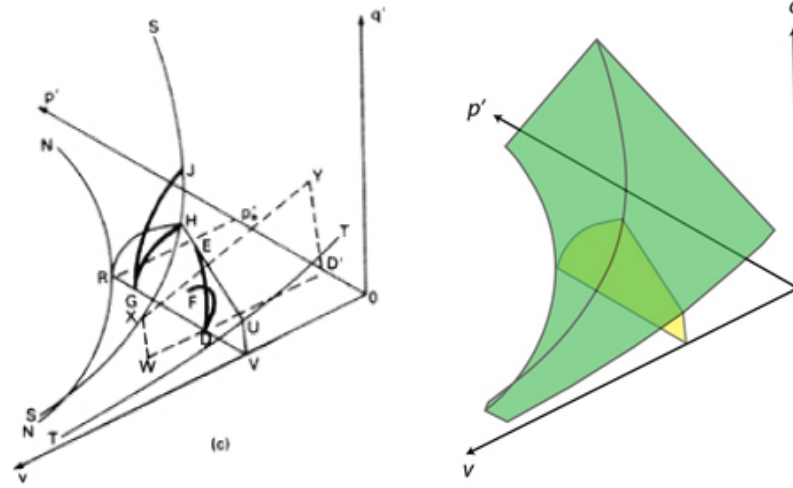


Figure 3.5: The critical state concept for normally and over consolidated clays Craig [2004]. The right hand figure shows the state surface boundary in 3D (green) and for constant volume conditions (yellow).

stress) is exceeded and plastic deformation prevails [Schofield and Wroth, 1968].

At stress conditions within the failure envelope i.e. $F < 0$, the volumetric behaviour is elastic and defined by the gradient of the slope for recoverable power per unit volume (κ -line in Figure 3.6). In the Cam Clay formulation this represents non-linear elasticity due to the non-linear relationship between volume change and applied load and therefore appears as a straight line on a plot of void ratio *vs* log net mean stress [Schofield and Wroth, 1968]. It describes the non-linear elastic response to both loading and unloading in terms of the elastic strain energy that can be recovered during compression-unloading cycles. Recoverable power per unit volume in general is given by:

$$-\left(\frac{p\Delta v_a^r}{v_a} + q\epsilon^r\right) \quad (3.14)$$

where v_a is the specific volume of the sample, and the superscript r denotes a recoverable process [Schofield and Wroth, 1968]. Making the assumption that shear strains are non-recoverable, the recoverable power per unit volume of a sample is given by:

$$-\left(\frac{p\Delta v_a^r}{v_a} + q\epsilon^r\right) = \frac{\kappa\Delta p}{v_a} \quad (3.15)$$

The relation to the applied load and any loss of energy through friction is then given by:

$$\frac{p\Delta v_a}{v_a} + q\Delta\epsilon - \frac{\kappa\Delta p}{v_a} = Mp|\Delta\epsilon| \quad (3.16)$$

where $\frac{p\Delta v_a}{v_a} + q\Delta\epsilon$ is the applied load, $\frac{\kappa\Delta p}{v_a}$ is the recoverable energy, and $Mp|\Delta\epsilon|$ is the frictional loss [Schofield and Wroth, 1968].

The plastic response is the remainder of the applied load that is dissipated through the specimen during plastic deformation and is defined by the difference in void ratio of the sam-

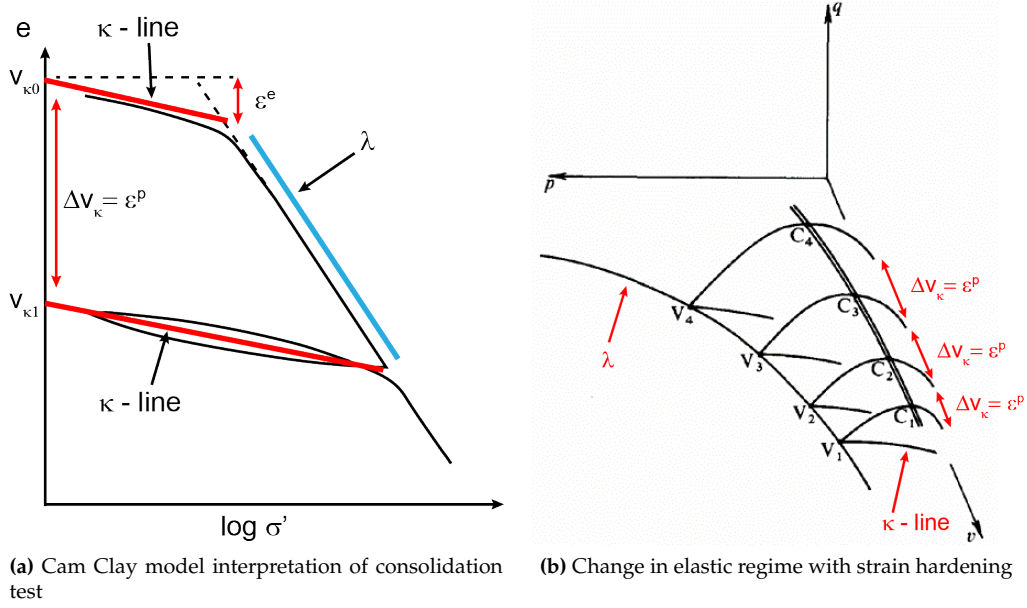


Figure 3.6: (a) Graphical representation of the Cam-Clay method showing a typical one-dimensional consolidation test interpreted in light of the Cam-Clay model in which the recoverable strains are described by the recoverable strain energy and the non-recoverable strains described by the energy dissipated within the system. (b) The increase in pre-consolidation pressure with decreasing volume caused by strain hardening as a result of plastic unrecoverable strains (after [Schofield and Wroth, 1968]).

ple at a given stress on the loading and unloading path (ϵ^p in Figure 3.6a) [Schofield and Wroth, 1968]. It can be defined in general in terms of the non-recoverable power per unit volume as:

$$\frac{p \Delta v_a^p}{v_a} + q \Delta \epsilon^p \quad (3.17)$$

where the superscript p denotes plastic behaviour [Schofield and Wroth, 1968]. Plastic deformation results in the permanent movement of the κ -line with respect to void ratio and enables strain hardening and strain softening to be modelled by the change in the yield stress or pre-consolidation pressure ($V_1 - V_4$ in Figure 3.6b). Plastic volumetric changes under loading are governed by the slope of the virgin consolidation curve (λ) e.g. in Figure 3.6a.

Loading past the pre-consolidation pressure reduces the volume of the sample and increases the pre-consolidation pressure required in subsequent deformations. Increments of plastic loading therefore change the size of the elastic regime but do not change the gradient of the κ -line, implying that the non-linear elastic response of the sample is the same in loading and unloading. Figure 3.6(b) shows the change in the size of the non-linear elastic regime as a function of the volume of the sample [Schofield and Wroth, 1968]. As volume decreases the pre-consolidation pressure increases due to strain hardening induced by non-recoverable strains. The energy of the applied load that cannot be recovered in volumetric strains is transferred into strain hardening i.e. increasing the yield strength of the material.

In order to fully describe the behaviour of a soil, information regarding the gradient of the κ -line, the virgin consolidation curve (λ), and the pre-consolidation pressure are required. Commonly these are calibrated to one dimensional consolidation tests. The modified cam-clay approach is widely used, and while it is not specific to the behaviour of expansive soils

such as bentonite, it successfully manages to recreate the observations such as strain hardening/softening and pressure sensitivity [Borja and Lee, 1990]. The Cam Clay models are able to predict behaviour quite successfully, but do not aim to address the physical processes occurring in the bentonite. Furthermore, the model is a description of the mechanical behaviour only, and therefore does not include any dependence on the hydraulic process and properties such as suction.

In order to take into account the close coupling between the hydraulic and mechanical processes observed in unsaturated bentonite, constitutive frameworks relate the failure criteria to the hydraulic suction. The most commonly used of these frameworks are the Barcelona models developed by Alonso et al. [1990, 1999], Gens and Alonso [1992], Navarro et al. [2014], Sánchez et al. [2005], although alternative formulations have also been proposed based on different choices of stress variables e.g. Wheeler and Sivakumar [1995].

3.1.3.2 The Barcelona Models

The Barcelona models have been developed as bottom-up style models of clay behaviour that are primarily concerned with expressing all structural scales and their control on the overall medium behaviour [Alonso et al., 1990]. The original Barcelona Basic Model (BBM) was developed to model behaviour of non-expansive/limited expansivity soils and led to the development of the Barcelona Expansive Model (BExM) for highly expansive soil behaviour [Alonso et al., 1999, Gens and Alonso, 1992, Sánchez et al., 2005].

Both the BBM and BExM are extensions of the modified Cam Clay model to include the dependence of the soil suction on the mechanical behaviour of the soil [Alonso et al., 1990, Gens and Alonso, 1992]. Numerous experimental results have shown an increase in the pre-consolidation pressure with suction including the SEALEX experiments modelled in this work [Wang, 2012]. In the Barcelona models, the modified Cam Clay yield surface is defined in terms of net mean stress (p) and deviatoric stress (q) as usual, and combined with a third stress variable of suction (s) to describe the full yield surface, as shown in Figure 3.7 [Alonso et al., 1990, 1999, Gens and Alonso, 1992]. The yield surface in $p - s$ space is termed the Loading-Collapse (LC) curve and defines the volumetric behaviour under a mechanical load (Loading) or a reduction in suction (Collapse). The LC curve can be conceptualised as a variation in pre-consolidation pressure with suction and visualised as the surface linking the pre-consolidation pressure of multiple consolidation tests on identical samples at different suctions [Agus, 2005, Gens and Alonso, 1992] (Figure 3.7). It can be described mathematically from the following equation:

$$p_0 = p_c \left(\frac{p_0^*}{p_c} \right)^{\frac{\lambda(0) - \kappa}{\lambda(s) - \kappa}} \quad (3.18)$$

where p_0^* is the saturated yield stress (Pa), p_c is the reference net mean stress (Pa), $\lambda(0)$ is the slope of the virgin consolidation line at saturation, $\lambda(s)$ is the slope of the virgin consolidation curve for the suction (s), and κ is the slope of the elastic compression index [Alonso et al., 1999].

The dependency of the slope of the virgin consolidation curve on the suction is given by an asymptotic relationship:

$$\lambda(s) = \lambda(0) \left[(1 - r_{max}) \exp(-\beta s) + r \right] \quad (3.19)$$

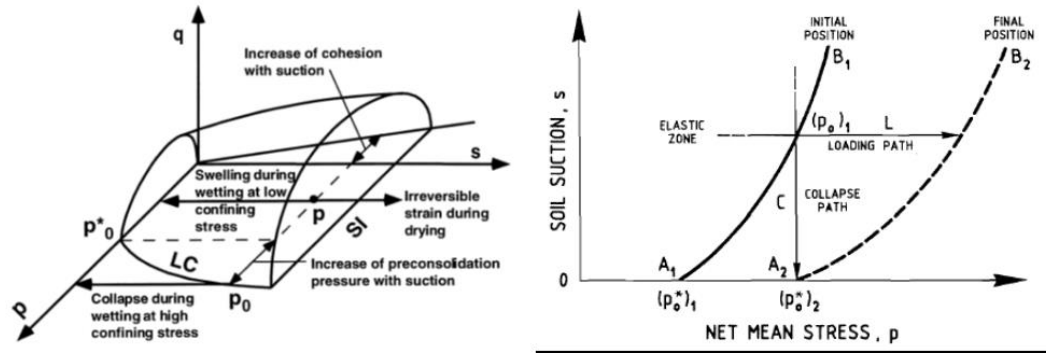


Figure 3.7: Left: A three-dimensional representation of the yield surface in the BBM and BExM models Alonso et al. [1999]. Right: A two-dimensional representation of the Loading-Collapse curve (LC on left diagram) Gens and Alonso [1992]

where r_{max} is related to the maximum stiffness the soil could have, and β_s determines the rate of how much stiffer the soil becomes with increasing suction [Alonso et al., 1990].

The shape of the LC curve and the size of the yield surface represents the observation that the pre-consolidation pressure for unsaturated soils increases with higher suctions [Sánchez et al., 2005]. This concept is termed ‘suction hardening’ and has its basis in the interpretation that increasing suction leads to increasing grain contact and interface action which results in greater apparent cohesion [Nuth and Laloui, 2008]. Suction hardening upon drying clearly implies a process of suction softening upon hydration, which is thought to be the cause of wetting- induced collapse; the suction softening decreases the size of the yield surface whilst continued hydration causes an increase in mechanical stress until the yield surface is reduced enough or enough stress is built up to cause plastic yielding [Sheng et al., 2008]. Reaching this yield surface causes the onset of plastic behaviour and irreversible volumetric change.

However, the early versions of the BBM considered the hydraulic behaviour to be represented by a state surface because the mechanical model was determined with respect to changes in net stresses and was not directly coupled to the hydraulic process [Gens et al., 2006]. In order to consider a direct coupling, whereby the hydraulic process is able to cause a change in the mechanical behaviour, specific attention to the inclusion of the hydraulic process in the constitutive model was required [Gens et al., 2006]. Houlsby [1997] determined that the overall work balance of an unsaturated soil could be described by the work required to compress the air phase, the work required to cause a change in saturation, and the work required to cause a change in average deformation. This led to the inclusion of a hydraulic component into the elasto-plastic constitutive models so that the overall work of the system was described by an effective mechanical stress that brings about a skeletal strain, and a hydraulic stress (suction) that brings about a change in saturation scaled by the porosity [Gens et al., 2006, Houlsby, 1997]. Incorporation of the hydraulic process in the constitutive framework requires the consideration that the stress state is a function of both the hydraulic and mechanic properties as suggested by Houlsby [1997]. Consequently additional failure curves, known as the Suction Increase (SI) and Suction Decrease (SD) failure curves, were defined for the development of the BExM and other constitutive models [Gens et al., 2006, Wheeler and Sivakumar, 1995]. Furthermore, experimental evidence indicating the presence of a bi-modal pore size distribution and the interaction between the micro-and macro-porosity led to the

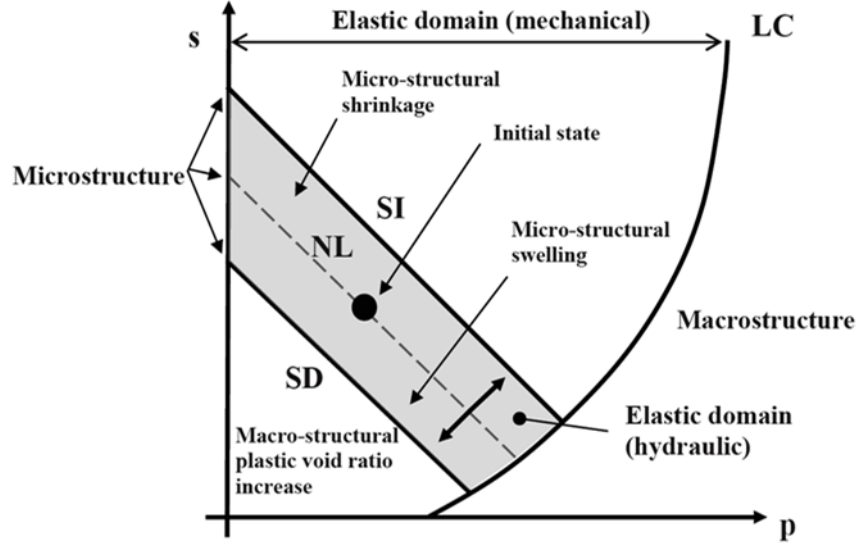


Figure 3.8: A graphical representation of the LC curve and the NL curve [Alonso et al., 1999]

development of the BExM that considers both structural scales.

The interaction between the micro-structure and macro-structure is incorporated into the Barcelona Expansive Model by considering strain to be partitioned between the two structural scales. Deformation of the micro-structure is considered to be fully reversible and unaffected by macro-structural strains, whereas deformation of the macro-structure can be both elastic and plastic and can also be influenced by the micro-structural strains. The elastic strain of the micro-structure (ϵ_{vm}^e) is given by:

$$d\epsilon_{vm}^e = \frac{\kappa_m}{(1 + e_m)} \frac{d\hat{p}}{\hat{p}} \quad (3.20)$$

where κ_m is the compression index for the micro-structure, e_m is the micro-structural void ratio, and $\hat{p}$ is a micro-structural effective stress. The micro-structure is considered to be saturated at all times and therefore deformation occurs as a result of changes to the effective stress i.e. specific consideration of the influence of suction or net mean stress separately is not necessary for the micro-structure. The application of the effective stress concept to the micro-structure gives rise to a line at which no volumetric strain will occur in the micro-structure. This is termed the Neutral Line (Figure 3.8) [Alonso et al., 1999]. Elastic strain of the macro-structure ϵ_{vM}^e on the other hand is dependent on the individual influences of suction and net mean stress and is given by:

$$d\epsilon_{vM}^e = \frac{\kappa}{(1 + e_M)} \frac{dp}{p} + \frac{\kappa_s}{(1 + e_M)} \frac{ds}{s + p_{atm}} \quad (3.21)$$

where κ and κ_s are the compressive indices in an e -log(p) and e -log(s) plot respectively, and p_{atm} is the atmospheric pressure [Alonso et al., 1999].

Plastic deformation under isotropic conditions in the BExM follows the virgin consolidation curve, which is defined as:

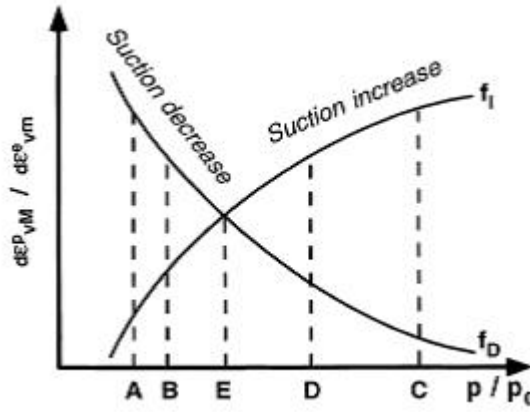


Figure 3.9: Typical coupling functions of microstructure swelling or shrinkage [Alonso et al., 1999]

$$d\epsilon_{vp} = -\lambda(s) \frac{dp}{p} \quad (3.22)$$

where $\lambda(s)$ is the slope of the virgin consolidation line at the suction (s) [Agus, 2005]. The virgin consolidation curve for suction changes is defined as:

$$d\epsilon_{vs} = -\lambda_s(p) \frac{ds}{(s + p_{atm})} \quad (3.23)$$

where λ_s is the stiffness parameter for the virgin soil at a given suction and is dependent on the net mean stress (p) [Alonso et al., 1990].

Plastic deformation affects only the macro-structural void ratio and can be brought about through a change in stress state to intersect the Loading-Collapse curve. It may also be caused by changes in suction which alter the stress state to intersect either Suction Increase or Suction Decrease failure curves [Alonso et al., 1999]. Primarily designed to allow direct incorporation of hydraulic hysteresis behaviour into the BBM model, these yield curves were also used in the BExM to model the stress conditions under which irreversible macro-structural strains occur as a result of suction changes [Gens and Alonso, 1992, Gens et al., 2006]. These failure criteria are activated when the NL line intersects with either one through changes in micro-structural effective stress, and delimit the hydraulic conditions under which elastic volumetric changes can occur [Alonso et al., 1999]. Incremental macro-scale volumetric plastic strain is expressed in the BExM as an interaction of two functions that describe the plastic behaviour during micro-structural swelling or shrinkage as shown in Figure 3.9 [Alonso et al., 1999, Sánchez et al., 2005]. The y axis is the ratio of the macro-structural plastic strain to the micro-structural elastic strain. The functions f_D and f_I are expressed as:

$$f_I = f_{I0} + f_{I1} \left(\frac{p}{p_0} \right)^{n_I} \quad (3.24)$$

$$f_I = f_{D0} + f_{D1} \left(1 - \frac{p}{p_0} \right)^{n_D} \quad (3.25)$$

where f_{I0} , f_{I1} , n_I , f_{D0} , f_{D1} , and n_D are all fitting parameters [Alonso et al., 1999].

In order to address the dependency of the swelling pressure and swelling strains on the ini-

tial state of the soil, the BExM modifies the location of the LC curve with respect to the dry density of the soil [Alonso et al., 1999]. Samples with a high dry density have low macro-structural void ratios. Therefore, assuming that the micro-structural behaviour is elastic, the irreversible volumetric changes incurred during loading only represent the change in the structure on the macro-scale. This is borne out by Mercury Intrusion Porosimetry tests that show the micro-structure is relatively unaffected by compaction but the macro-structure is significantly altered [Lloret et al., 2003, Ye et al., 2009]. A high density sample, therefore, will exhibit more elastic behaviour and less plastic behaviour, so the size of the yield surface increases [Alonso et al., 1999].

The Barcelona models have become widely used in the scientific community for modelling expansive soils. However, the principle limitation of the models is the large number of parameters required to populate the model e.g. parameterisation of the BBM for a constant volume test in Navarro et al. [2015] requires 14 mechanical parameters.

3.2 Hydraulic models

The hydraulic process of bentonite hydration is commonly approached from two main angles; a Darcy type approach that makes use of the observation that flow is linearly related to a pressure gradient, and a physico-chemical approach based on electrolyte concentrations [Alonso et al., 1990, Liu, 2010, Liu et al., 2009, 2011, Nguyen et al., 2005]. In this work the former approach is applied and as such the key features of these hydraulic models are discussed.

3.2.1 Water retention curve models

The water retention curve is fundamental to the simulation of the hydraulic behaviour of an unsaturated soil as it defines the change in hydration state of the soil via the constitutive relationship between suction and water content or degree of saturation [Fredlund, 2002]. It is determined experimentally either under constant volume conditions or in free swell conditions, and is the combination of the measured suction of a sample and the measured gravimetric water content. Typically in non-expansive soils this data is then converted to a relationship between suction and saturation that is used directly in Darcy-based hydraulic solutions for unsaturated flow, such as Richards' equation.

3.2.1.1 Experimental measurement

As described in Chapter 2 total suction is measured as the partial pressure of water vapour above the surface of the soil water (above the surface of the soil in experiment) relative to the partial pressure of water vapour above the surface of pure water. This relative vapour pressure is also known as the relative humidity [Fredlund et al., 2012]. Total suction is a combination of the effect of the soil structure on the relative humidity (matric suction) and the concentration of ions in the soil water (osmotic suction). Therefore the total suction of a sample can be controlled by subjecting it to varying degrees of relative humidity. There are two main methods to achieve this over large suction ranges; the vapour equilibrium technique for high suctions (e.g. >4.2 MPa) and the osmotic technique for low suctions (e.g. <8 MPa [Delage and Cui, 2008]). In the SEALEX experiments modelled in this study the vapour equilibrium technique was used for suctions >4.2 MPa and the osmotic technique for the suction range 0.01 MPa - 4.2 MPa [Wang, 2012] (Table 3.1).

In the vapour equilibrium technique the sample is placed in a desiccator above a saturated salt solution that imposes a specific suction on the sample. The osmotic technique requires the sample to be placed within a polyethylene glycol (PEG) solution at a given concentration to induce the required suction, and separated from direct contact with the solution by a semi permeable membrane [Delage and Cui, 2008, Wang, 2012]. Gravimetric water contents are determined by measuring the change in mass of the sample when at equilibrium with the imposed suction. Consequently, the experimentally determined water retention curve is made up of discrete measured points and in order to model the behaviour over the full range of suctions a function is required to express the change of water content with suction in a continuous manner.

Table 3.1: The experimental techniques used to determine the water retention curve by imposing discrete suctions and allowing the sample to equilibrate. Water content was then calculated from the increased mass of the sample at equilibrated conditions [Wang, 2012].

Suction control method	Solution	Suction (MPa)
Saturated Salt Solution	LiCl	309.00
	K ₂ CO ₃	113.00
	Mg(NO ₃) ₂	82.00
	NaCl	38.00
	(NH ₄) ₂ SO ₄	24.90
	ZnSO ₄	12.60
	KNO ₃	9.00
	K ₂ SO ₄	4.20
PEG Solution Concentration (g PEG/g Water)	0.302	1.00
	0.095	0.10
	0.030	0.01

3.2.1.2 Constant Volume-based water retention models

Water retention curve functions for non-expansive soils are commonly cast in terms of effective saturation and fitted with an empirical model [Helmig, 1997]. There are multiple examples of these, including the widely used gas-water models of Brooks and Corey, van Genuchten, and Fredlund and Xing [Fredlund and Rahardjo, 1993, Helmig, 1997]. The Brooks and Corey function is given by:

$$S_e(h) = \left(\frac{h_e}{h} \right)^{\lambda_p} \quad |h| > |h_e| \quad (3.26)$$

where S_e is the effective saturation, h is the fluid pressure (suction), h_e is the air entry pressure (also termed the bubbling pressure) and λ_p is a fitting function related to particle size distribution [Brooks and Corey, 1964]. A large λ value describes a sample of a single grain size, whereas a low λ value reflects a very non-uniform material [Brooks and Corey, 1964]. The van Genuchten model was developed to provide the pressure-saturation function for use in the estimation of unsaturated hydraulic conductivity from equations proposed by Mualem (1976a) [van Genuchten, 1980], and is given by:

$$\Theta = \frac{\theta_w - \theta_{res}}{\theta_s - \theta_{res}} = \left[\frac{1}{1 + (\alpha s)^{n_v}} \right]^m \quad (3.27)$$

where Θ is the water content that can be used to determine the effective saturation, s is the suction (Pa), α is a fitting parameter commonly related to the inverse of the air entry value (1/kPa), n_v is a fitting parameter related to the particle size of the soil, and m is a constant approximated by:

$$m = 1 - \frac{1}{n} \quad (3.28)$$

The Fredlund and Xing [1994] model is given by:

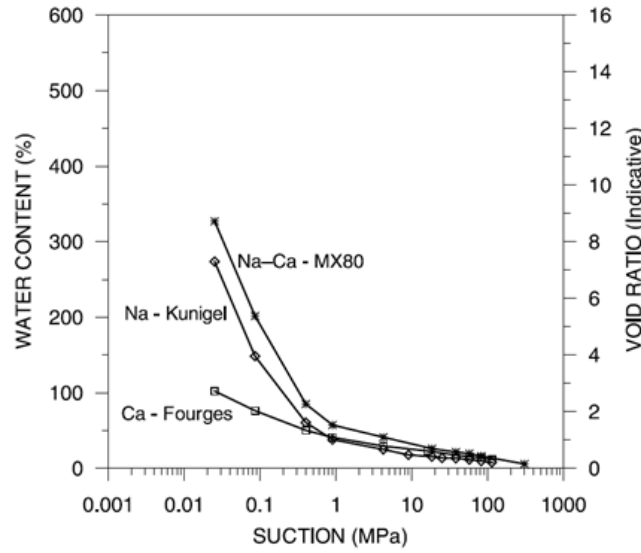


Figure 3.10: Water retention curves for three different bentonite powders showing a typically bi-model relationship between suction and water content (a). Also plotted in (a) is the void ratio showing the increase in volume of the sample with a decrease in suction [Marcial et al., 2002].

$$\Theta = \frac{\theta_w}{\theta_s} = \theta_w = C(s) \frac{1}{\left\{ \ln \left[\exp(1) + \left(\frac{s}{a} \right)^n \right] \right\}^m} \quad (3.29)$$

where a is a fitting parameter that is a function of the air entry value, and the correction factor ($C(s)$) is given by:

$$C(s) = 1 - \frac{\ln \left(1 + \frac{s}{s_r} \right)}{\ln \left(1 + \frac{1000000}{s_r} \right)} \quad (3.30)$$

where s_r represents the suction corresponding to the residual volumetric water content [Agus, 2005].

Although developed on non-expansive soils, under constant volume conditions water retention functions such as the van Genuchten formula are also suitable for calculating the hydraulic properties of expansive soils because the final degree of saturation can be determined from the finite volume of the constrained sample. However, expansive soils under free swelling conditions have different soil water retention characteristics and due to their volumetric behaviour require special consideration. For example Marcial et al. [2002] report a typically bi-modal water retention curve for both Na^+ and Ca^{2+} bentonite samples under free swell conditions with gravimetric water contents in excess of 300% for MX-80 bentonite (Figure 3.10). The same behaviour is observed in the SEALEX experiments that provide the data for this modelling work (Figure 3.11) [Wang, 2012]. In free swell conditions the volumetric change caused by hydration can lead to a change in pore shape and connectivity, as shown in Figure 2.10 in Chapter 2. Furthermore, the degree of saturation in free swell conditions constantly evolves with increasing volume. As a result the water retention curve functions require the volumetric dependency of the water retention curve to be considered for expansive soils [Gallipoli et al., 2003].

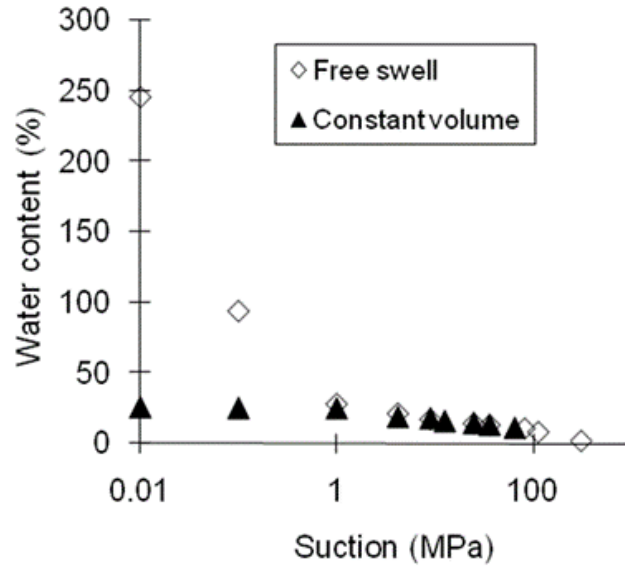


Figure 3.11: Water retention properties determined during the SEALEX experiments under constant volume and free swell conditions. There is a significant difference in water retention behaviour between the two stress conditions [Wang, 2012] with the free swell results exhibiting a typically bi-modal behaviour.

Gallipoli et al. [2003] present a method of adjusting the van Genuchten equation to include a dependency on specific volume of the sample. This is achieved via a modification to the fitting parameter α in Equation 3.27 given by:

$$\alpha = \phi e_g^\psi \quad (3.31)$$

where ϕ and ψ_g are soil constants, and e is the void ratio. This results in the volume dependent van Genuchten function taking the form [Gallipoli et al., 2003]:

$$\Theta = \left\{ \frac{1}{1 + [\phi e_g^\psi s]^n} \right\}^m \quad (3.32)$$

This formulation has been used in elasto-plastic formulations where the change in void ratio is calculated via the mechanical constitutive framework (e.g. D’Onza et al. [2011], Gallipoli et al. [2003]) to model the volumetric dependency of the water retention curve. Further advances to these models have included the hydraulic hysteresis to define bounding surfaces for both drying and wetting paths (e.g. [Gallipoli et al., 2015, Tsiampousi et al., 2013]). The work in this thesis models a suite of experiments with a single hydration phase and as such is primarily concerned with the wetting path. It therefore does not consider hysteresis.

The models described so far to characterise the water retention properties of an unsaturated soil start from a function derived for constant volume conditions and aim to adjust for volumetric changes in unsaturated soils. This approach could satisfactorily reproduce the constant volume water retention behaviour shown in Figure 3.11 but requires a sophisticated hydro-mechanical model to accurately calculate the volume change in order to determine the free swell water retention behaviour also presented in Figure 3.11. Similarly the indirect coupling of the soil water retention properties to the stress has implications for the constitutive

framework used to describe the stress state. The dependence of the stress on the hydration state is required to be defined in order to determine the stress-state of the overall sample, and consequently many constitutive model frameworks applied to unsaturated soils consider the two independent stress variables approach, as proposed by Fredlund and Morgenstern [1977].

3.2.1.3 Free swell-based water retention models

For the case of unsaturated soils an alternative approach was first presented by Croney et al. [1958] and later developed by Dueck [2004]. As opposed to starting with a constant volume function and calculating the effect of volume change on water retention properties, this approach calculates from the free swell water retention behaviour and then determines the water retention behaviour at any state of confinement between free swell and constant volume conditions as a function of the confining stress. This approach has been termed Dueck suction in this work and is defined in terms of mean net stress as:

$$P(RH, w_f) = -\frac{R \cdot T}{v_w \cdot \omega_v} \cdot \ln \left(\frac{RH_{ret}(w_f)}{RH} \right) \quad (3.33)$$

where P is the mean total stress (Pa), R is the universal gas constant (J/(mol K)), T is the temperature ($^{\circ}\text{K}$), v_w is the specific volume of water (m^3/kg), ω_v is the molecular mass of water vapour (kg/kmol), RH is the measured relative humidity (-), w_f is the water content (-), and $RH_{ret}(w_f)$ is the relative humidity from the retention curve as a function of the final water content in free swell conditions [Dueck and Börgesson, 2007]. Equation 3.33 calculates the mean total stress as a function of the measured suction and the free swell suction at a given water content. This concept is best illustrated by Figure 3.12 which shows that the water retention properties of a constant volume or partially confined sample can be determined from the free swell retention data as a function of the mean total stress. This can also be expressed simply as:

$$s_c = s_{fs} - \sigma_c \quad (3.34)$$

where s_c is the suction in any state of confinement between constant volume and free swell conditions (Pa), s_{fs} is the free swell suction determined experimentally (Pa), and σ_c is the confining stress (mean total stress) (Pa) [Dueck, 2004, Dueck and Börgesson, 2007].

This formulation has the advantage that the stress is directly incorporated into the calculation of the hydraulic properties of the sample and the implications are two fold;

- Firstly, the effect of large expansive volume changes are inherently incorporated into the water retention model as the free swell curve defines the maximum water uptake for a given suction at zero confining stress,
- Secondly, there is a dependence of the hydration state on the stress state of the sample and therefore a similar dependence of the stress state on the hydration state of the sample. This, therefore, provides a mechanism to incorporate the coupling required to complete the stress state when a single value effective stress concept is applied i.e. Bishop's effective stress.

However, the concept of Dueck suction only applies to stress conditions ranging from constant volume to free swell. This is because the relationship between stress, suction, and water

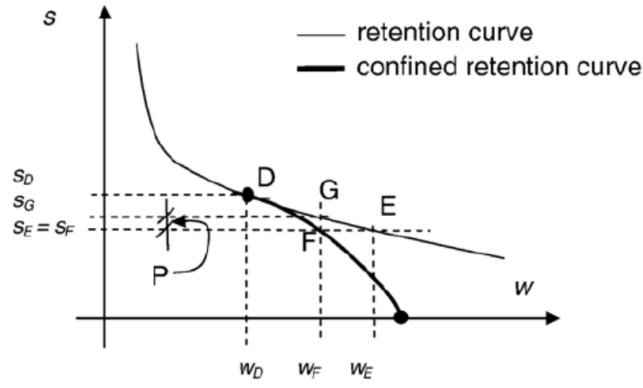


Figure 3.12: Graphical representation of the Dueck suction concept after [Dueck, 2004, Dueck and Börgesson, 2007]. ‘Retention curve’ represents the free swell water retention data determined in experiment. In confined conditions less water is up-taken into the sample due to volumetric constraints imposed by the confining material. This generates a swelling pressure which corresponds to the difference between the free swell suction and the confined suction at a given water content.

content described by the Dueck suction model defines a type of state-surface for volume conditions equal to or greater than the initial conditions, and for confining stresses up to the developed swelling pressure [Gallipoli et al., 2003]. Non-reversible effects on the macro-structure of the sample during consolidation are not considered and therefore, in standard soil mechanics consolidation tests, the calculated water content is equal for a given value of stress irrespective of void ratio.

3.2.2 Permeability models

Applying a Darcy flow approach to the movement of fluid through bentonite requires a description of the ease with which fluid can pass through the medium. This is commonly termed the hydraulic conductivity and is a property of both the soil and the water;

$$K = \frac{\rho g}{\mu} k \quad (3.35)$$

where K is the hydraulic conductivity (m/s), ρ is the density of the fluid (kg/m³), g is the acceleration due to gravity (m/s²), μ is the viscosity (Pa·s) and k is the intrinsic permeability (m²). In deformable porous media such as an expansive soil where strains in excess of 100% are possible, the area available for flow (intrinsic permeability) evolves with the deformation. Furthermore, in unsaturated conditions the ease with which a fluid can flow through a sample is a function of the saturation. This phenomenon is expressed by a function known as the relative permeability.

3.2.2.1 Intrinsic permeability

A number of permeability models have been proposed for bentonites to take into account their volumetric tendencies, including statistical approaches [Agus, 2005], a model accounting for gel production [Pusch and Yong, 2003], empirical fits to data [Karnland et al., 2006] and variations on the Kozeny-Carmen equation such as the cluster model Achari et al. [1999] and

the ‘KC-like’ equation [Liu, 2010, Liu et al., 2011, Singh and Wallender, 2008].

3.2.2.1.1 Cluster Model

The cluster model aims to take into account the influence of clay aggregates on the permeability through the electrochemical effect of the adsorption of water to aggregate surfaces. It is therefore mainly applicable for clay compositions in which the Gouy-Chapman diffuse double layer theory holds i.e. dry densities lower than $c.1.55 \text{ Mg/m}^3$ [Alonso et al., 1999, Komine and Ogata, 1996]. Consequently, it is not compatible with the range of dry densities investigated in this work. Furthermore it requires the separation of void ratio into that of the micro-structure (intra-aggregate) and the macro-structure (inter-aggregate) which would further require separate water retention curves to be parameterised [Alonso et al., 2011, Gens et al., 2011, Navarro et al., 2015], and requires many iterations to determine inter-particle stresses corresponding to the load conditions [Achari et al., 1999, Liu, 2010].

3.2.2.1.2 Gel Model

The gel model derived by Pusch and Yong [2003] aims to reflect the experimental observations that the bentonite structure is composed of clay aggregates and gel within the interconnecting pores during hydration. In order to determine the coefficient of permeability a digital micro-graph of the sample is required to estimate the density of the gel and the aggregates, which is then used in combination with the number of channels parallel to and perpendicular to the flow direction to give an average permeability for a given element [Pusch and Yong, 2003].

3.2.2.1.3 Kozeny-Carmen Model

It has been noted that the Kozeny-Carmen model is most effective for non-plastic granular materials [Achari et al., 1999, Liu, 2010] but is not as successful in predicting the saturated permeability of bentonite. The Kozeny-Carmen equation determines the permeability of a porous medium as a function of the porosity, the specific surface, and the Kozeny constant that reflects the pore-shape and tortuosity of flow channels [Liu, 2010]. Written in terms of volume fraction the K-C equation is:

$$k = \frac{1}{k_0 \tau_a^2 a_p^2} \frac{(1 - \phi_k)^3}{\phi_k^2} \quad (3.36)$$

where k_0 is the pore-shape factor, τ_a is the tortuosity of flow paths, a_p is the specific surface area per unit volume of particles, and ϕ_k is the volume fraction of the solid to liquid [Liu, 2010]. Clearly the specific surface and pore-shapes are likely to be significantly different for expansive clay materials compared to well sorted, well rounded sandstones.

3.2.2.1.4 Empirical formulas e.g. Karnland et al. [2006]

The sample dry density has a major control over the hydro-mechanical properties of bentonite such as the swelling pressure and so, in order to relate permeability to dry density, Karnland et al. [2006] derived an empirical formula for intrinsic permeability of the form:

$$k = \alpha_k e^{\beta_k \rho_d} \quad (3.37)$$

where α_k is the permeability (m^2) at a bentonite dry density of 0.0 i.e. the y intercept of a log permeability- dry density graph, e is the exponential function, β_k is a fitting function, and ρ_d is the bentonite dry density (kg/m^3) [Karnland et al., 2006].

3.2.2.1.5 KC-like Model after Liu [2010], Liu et al. [2011]

Following analysis of measured permeability values Liu [2010] identified that the Kozeny 'constant' ($k_0\tau^2$) is not in fact constant for Na^+ bentonites but increases with increasing volume fraction. This could be the reason for the KC equation not reproducing the experimental results. Liu [2010] report that Carmen identified this in his experiments and interpreted this as a result of water held on the surface of the clay that is not available for flow and reduces the space within which flow can occur. Liu [2010] further reasoned that the ionic concentration of the hydrating fluid does not significantly influence the permeability and therefore development of a KC-like equation need not necessarily include the electrochemical effect of diffuse double layers as proposed by the cluster model [Achari et al., 1999]. In order to account for the deviation of the permeability from the Kozeny constant Liu [2010] proposed an edit to the KC equation that considers the sheet-like grain shape of montmorillonite and the mass fraction of montmorillonite within the bentonite or bentonite-sand mixture [Liu, 2010, Liu et al., 2011]:

$$k = \frac{\delta_p^2}{4C_k\zeta_p^2} \frac{(1 - \phi_k)^{m_a}}{\phi_k^l} \quad (3.38)$$

where δ_p is the average particle thickness of a montmorillonite sheet (nm), C_k is considered to be the scaled pore shape factor that is a combination of $k_0\tau_a^2$, ζ_p is the mass fraction of montmorillonite within the solid grains, ϕ_k is the volume fraction of the solid, and m_a and l are calibrating model parameters that determine the dependency of the intrinsic permeability on the solid volume fraction. When m and l are equal to 3 and 2 respectively, the function is equivalent to the conventional K-C equation. The volume fraction of the solid is related to the porosity (n) by:

$$\phi_k = 1 - n \quad (3.39)$$

The mass fraction (ζ_p) in the Liu et al. [2011] model refers to the mass fraction of the montmorillonite with respect to the solids in the sample. The function calculates a permeability that is effectively a function of the dry density and porosity of the material and is therefore applicable to the volumetric changes associated with bentonite hydration under free swell conditions. C_k and δ_p may be estimated from the average values used in Liu et al. [2011], and m and l can be calibrated to experimental results.

3.2.2.2 Relative permeability

Intrinsic permeability accounts for the area available for flow within a sample and is determined for a saturated soil. For unsaturated soils the pore space is filled with both air and water, and the presence of two fluids within the pore space affects flow. Due to the capillary effect in larger pore spaces, the wetting fluid is preferentially attracted to the grain surfaces and the non-wetting fluid occupies the central areas of larger pores [Craig, 2004, Helmig, 1997]. In bentonite the internal suction of the montmorillonite adds to this process by attracting water molecules to the grain surfaces and within the crystal structure. Therefore, the area available

for flow of the wetting fluid (e.g. water) is reduced by a factor related to the saturation of the pore space, and the flow paths for the wetting fluid around the edges of the pores increase in length i.e. there is an increase in tortuosity of flow paths [Helmig, 1997]. To account for this, a factor termed the relative permeability is defined. This is the ratio between the effective permeability in a system containing more than one fluid and the permeability of a system containing only one fluid [Brooks and Corey, 1964]:

$$k_{rel} = \frac{k_e}{k} \quad (3.40)$$

where k_{rel} is the relative permeability, k_e is the effective permeability of a sample containing more than one fluid, and k is the permeability of a sample saturated with one fluid i.e. the intrinsic permeability [Brooks and Corey, 1964]. Commonly used relative permeability functions include the Brooks and Corey [1964] and van Genuchten [1980] models that combine the respective pressure-saturation relationships with a pore network model [Helmig, 1997]. The Brooks and Corey [1964] model determines the relative permeability as a function of saturation and an empirical constant related to the pore size distribution:

$$k_{rel} = S^\eta \quad (3.41)$$

where S is the saturation, and η is the empirical constant related to the pore size distribution parameter λ_p by:

$$\eta = \frac{2 + 3\lambda_p}{\lambda_p} \quad (3.42)$$

For soils with uniform pore size distribution the value of λ_p is large and results in a smaller empirical constant for relative permeability. On the contrary soils with a very varied grain size distribution have a low value of λ_p and a correspondingly high relative permeability empirical constant [Brooks and Corey, 1964, Fredlund et al., 2012].

The van Genuchten [1980] model calculates the relative permeability of the wetting phase from:

$$k_{rel} = S_e^{\epsilon_v} \left[1 - (1 - S_e^{\frac{1}{m}})^m \right]^2 \quad (3.43)$$

where the parameters are the same as used in the pressure-saturation function (Equation 3.27), and ϵ_v and γ_v are empirical functions to describe the connectivity of the pore network [Helmig, 1997].

Chapter 4

Mathematical Model of the Hydro-Mechanical system

The hydro-mechanical behaviour of bentonite is a strongly coupled phenomenon. As a result, the simulation and prediction of the system behaviour relevant to industrial applications requires a model capable of accounting for the strong interaction between hydraulic fluid flow and either mechanical deformation, or stress build-up. In this chapter a coupled hydro-mechanical model based on Richards' equation for unsaturated fluid flow and a mechanical framework of non-linear elasticity are presented. A moving finite element mesh is developed and incorporated into the mechanical and hydraulic solutions in order to inform the material non-linearity in the mechanical model, and to ensure consistency within the coupling to the hydraulics. Each process is addressed separately from a theoretical point of view followed by the main implementations and developments in the code. The coupling between the hydraulics and mechanics is then discussed before the moving mesh application is presented. The following chapters (5, 6, and 7) present and discuss the results of the application of this model to the SEALEX experiments. The model is developed in the open source, object oriented finite element code OpenGeoSys [Kolditz et al., 2012].

4.1 OpenGeoSys

OpenGeoSys (OGS) is an open source initiative designed to encourage a collaborative research effort to develop coupled process models for Thermal-Hydro-Mechanical-Chemical (THMC) applications [Kolditz et al., 2012]. The code has been developed by a collaboration of developers from different institutions and has seen a progression from the original RockFlow in Fortran in the 1980's, to RockFlow-C in C and GeoSys/RockFlow in C++, through to the latest OpenGeoSys release version- OGS-5.5.7 in C++ [Kolditz et al., 2012, www.opengeosys.org]. The object-oriented code allows the calculation and coupling of a range of processes and provides the flexibility to combine and implement different constitutive models for coupled processes.

Figure 4.1 shows the file structure of the object oriented code [Kolditz et al., 2012]. In order to complete a process that solves the governing equations, the relevant input files are required. MSH refers to the finite element mesh that can be generated via an independent

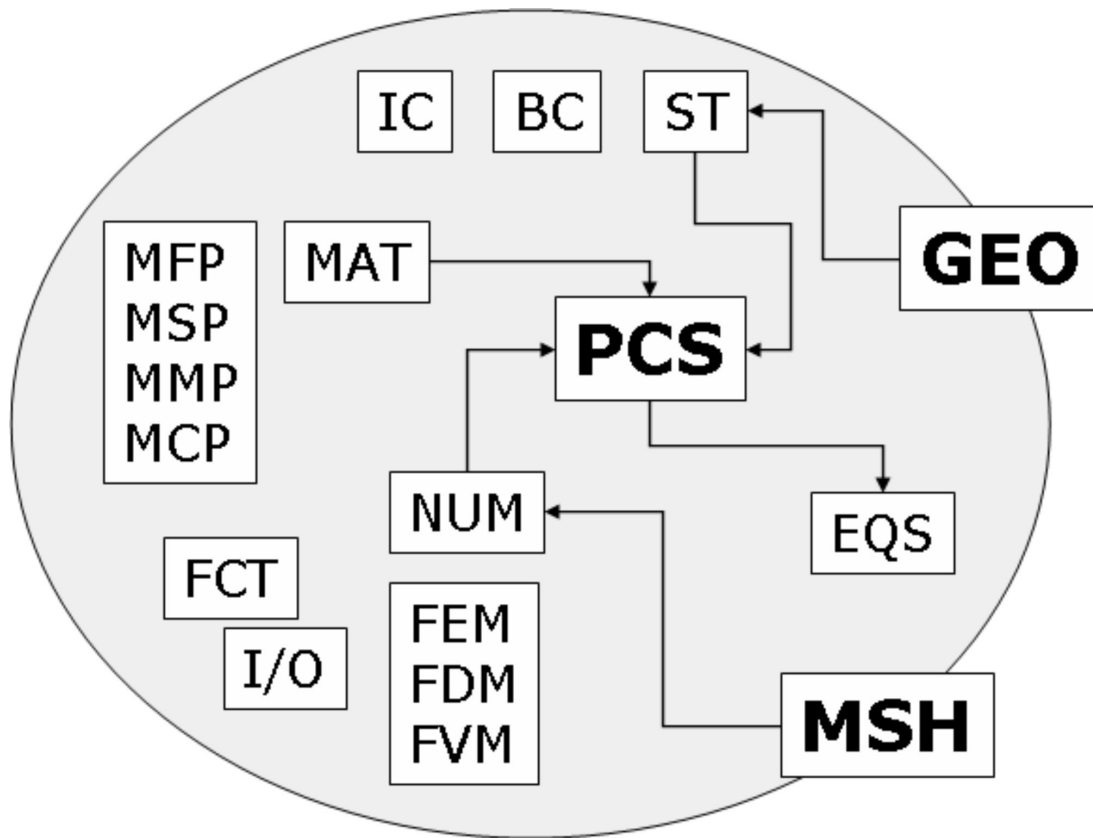


Figure 4.1: The file structure and necessary inputs required to run a model in the object oriented code OpenGeoSys [Kolditz et al., 2012]

mesh generating software e.g. Gmsh [Geuzaine and Remacle, 2009] and imported into OGS. The mesh is made of nodes and elements, over which the governing equations of the process are calculated and interpolated. The geometry object (GEO) is required to identify points, lines or surfaces in the model that can be used to apply boundary conditions (BC), source terms (ST), initial conditions (IC), and/or data output (I/O). Information regarding the properties of the modelled material is input into the model via the material properties relevant to the modelled process e.g. fluid properties (MFP), solid properties (MSP), and medium properties (MMP) are required for a hydro-mechanical coupled model [Kolditz et al., 2012]. Chemical properties (MCP) would be required for a mass transport or reactive transport process. The solving method, accuracy criteria, and coupling conditions are defined in the numerics file (NUM). Finally the process class (PCS) manages the combination of these objects to construct the equation systems that can be solved in order to simulate the process [Kolditz et al., 2012].

4.2 Hydraulic Model - Theory

Modelling the re-saturation of bentonite requires the consideration of hydraulic flow through an unsaturated medium with porosity on multiple scales and strong physico-chemical forces acting between the solid matrix and the pore fluid. This complex scenario can fortunately be greatly simplified from a hydraulic point of view because fluid flow remains suction pressure driven and can therefore be approximated by the Darcy's law of pressure driven flow

[de Marsily, 1986]:

$$Q = AKi \quad (4.1)$$

where Q is the volumetric flow rate (m^3/s), A is the cross-sectional area (m^2), K is the hydraulic conductivity (m/s), and i is the hydraulic gradient (-) which expresses the pressure gradient driving fluid flow.

For this application, however, the specific considerations of a partially saturated medium need to be considered. The system comprises at least two fluid phases; water and gas. It can therefore be considered a multiphase system and can be described by full multiphase fluid flow. In these conditions the degree to which the sample is saturated with each fluid phase becomes important for the ability for each fluid phase to flow. The overall saturation of the pore space is unable to exceed 100% so the averaging method of considering multiphase flow requires that the saturations of all fluid phases sum to equal 100%. In true multiphase flow each component of the gas may be considered an individual phase in itself with differences in gas pressure arising from the flow of each component. However, for simplicity's sake during the development of this model, the simpler assumption that the gas pressure remains constant throughout the system is adopted. This is commonly referred to as Richards' approximation [Celia et al., 1990].

4.2.1 Unsaturated Flow

The basis of Richards' approximation is the assumption that the gas pressure is constant throughout the system and can be left out of the governing equations of fluid flow i.e. the gas pressure has no influence on the flow of the fluids and is reflected in the equations through the degree of saturation of the fluid phase. Richards' equation can be derived from the conservation of mass equation of a single fluid following Thorenz [2001]:

$$\frac{\partial(nS_\alpha\rho_\alpha)}{\partial t} + \text{div}(\rho_\alpha\mathbf{q}_\alpha) - \rho_\alpha Q_\alpha = 0 \quad (4.2)$$

where n is the porosity (-), S_α is the saturation of the fluid phase α (-), ρ_α is the density of the fluid phase (kg/m^3), $\mathbf{q}_\alpha$ is the Darcy velocity of the fluid phase (m/s), and Q_α is the production of the fluid phase or the source term (m^3/s) [Thorenz, 2001]. The Darcy velocity is a function of the gradient of fluid pressure (p_{c_α}) (Pa) and density (ρ_α (kg/m^3)) and gravity effects on the fluid ($\mathbf{g}$ (m/s^2)), the permeability tensor of the material ($\mathbf{k}$ (m^2)), the viscosity of the fluid (μ) (Pa.s), and the saturation dependent relative permeability (k_{rel}):

$$\mathbf{q}_\alpha = -\frac{k_{rel}\mathbf{k}}{\mu}(\text{grad } p_{c_\alpha} - \rho_\alpha\mathbf{g}) \quad (4.3)$$

This equation is comparable to that of saturated Darcy velocity except for the inclusion of the relative permeability factor (k_{rel}) [Thorenz, 2001]. The fluid mass conservation equation is determined by inserting equation 4.3 into equation 4.2 and expanding the time derivatives in the first term of the left hand side of 4.2 via the product rule [Thorenz, 2001]. This gives:

$$S_\alpha\rho_\alpha\frac{\partial n}{\partial t} + nS_\alpha\frac{\partial\rho_\alpha}{\partial t} + n\rho_\alpha\frac{\partial S_\alpha}{\partial t} - \text{div}\left(\rho_\alpha\frac{k_{rel}\mathbf{k}}{\mu}(\text{grad } p_{c_\alpha} - \rho_\alpha\mathbf{g})\right) - \rho_\alpha Q_\alpha = 0 \quad (4.4)$$

This mass conservation equation is converted into a volumetric form by assuming the porosity is non-deformable and that spatial changes in fluid density are far smaller than changes through time. The first term on the left hand side then becomes equal to 0 and the whole equation is divided by the fluid density to give;

$$\frac{nS_\alpha}{\rho_\alpha} \frac{\partial \rho_\alpha}{\partial t} + n \frac{\partial S_\alpha}{\partial t} - \frac{1}{\rho_\alpha} \text{div} \left(\rho_\alpha \frac{k_{rel\alpha} \mathbf{k}}{\mu_\alpha} (\text{grad } p_{c\alpha} - \rho_\alpha \mathbf{g}) \right) - Q_\alpha = 0 \quad (4.5)$$

This equation does not account for any compressibility effects of the gaseous phase or the matrix, so the term $\frac{nS_\alpha}{\rho_\alpha}$ is often replaced by a storativity term that reflects the compressibility of the whole soil. This soil storativity is given the term $S_{t\alpha}$. The temporal derivative of the density is also commonly replaced with the temporal derivative of the pressure such that the equation takes the form;

$$S_{t\alpha} S_\alpha \frac{\partial p_{c\alpha}}{\partial t} + n \frac{\partial S_\alpha}{\partial t} - \frac{1}{\rho_\alpha} \text{div} \left(\rho_\alpha \frac{k_{rel\alpha} \mathbf{k}}{\mu_\alpha} (\text{grad } p_{c\alpha} - \rho_\alpha \mathbf{g}) \right) - Q_\alpha = 0 \quad (4.6)$$

Replacing the temporal derivative of saturation with the product of the derivative of the capillary pressure function (i.e. the relationship between saturation and pressure) and the temporal derivative of the pressure results in Richards' approximation for partially saturated fluid flow;

$$\left(S_{t\alpha} S_\alpha + n \frac{\partial S_\alpha}{\partial p_{c\alpha}} \right) \frac{\partial p_\alpha}{\partial t} - \frac{1}{\rho_\alpha} \text{div} \left(\rho_\alpha \frac{k_{rel\alpha} \mathbf{k}}{\mu_\alpha} (\text{grad } p_{c\alpha} - \rho_\alpha \mathbf{g}) \right) - Q_\alpha = 0 \quad (4.7)$$

Richards' equation therefore defines a direct link between the saturation of the sample and the fluid pressure, which, in unsaturated samples, is termed the capillary pressure or suction pressure. This relationship can be experimentally derived and is commonly termed the water retention curve, suction curve, or soil-water characteristic curve [Fredlund, 2002]. The dependency of the solution on the relationship between suction pressure and saturation results in a non-linear equation where the calculated suction pressure is a function of the saturation, which in turn is a function of the suction pressure. In order to solve Richards' equation therefore, an iterative procedure is required e.g. a Picard iteration or Newton-Rapheson iteration [Istok, 1989]. Furthermore, this identifies the relationship between suction pressure and saturation to be a key parameter for the solution of unsaturated flow.

It should be noted that in the derivation of Richards' equation for unsaturated flow, Thorenz [2001] makes the assumption that the porosity is non-deformable and therefore simplifies the storage term by not considering the derivative of porosity with respect to time (Equation 4.4 to 4.5). However, bentonite is a highly expansive soil and the expectation is that during the hydration and swelling process the porosity will change. Nevertheless, this application of Richards' equation can still be valid because the change in porosity is a function of the mechanical solution i.e. deformation. Therefore, in order for the assumption to be valid in a staggered numerical scheme, it is necessary for the constitutive hydro-mechanical coupling model to account for this porosity change and incorporate the update of this variable throughout the hydraulic solution.

4.2.1.1 Finite Element Formulation of Richards Equation

Three main steps are required for a finite element approximation:

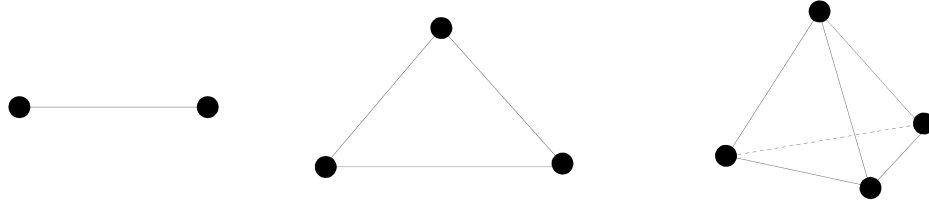


Figure 4.2: Examples of linear element shapes in one (bar), two (triangle) and three (tetrahedra) dimensions.

- Spatial discretisation of the problem domain.
- Discretisation of the integral form of the governing equations.
- Developing a system of equations using interpolation functions to approximate the unknown field variable values [Istok, 1989, Kolditz, 2002].

A brief description of each of these main steps is provided here. In depth discussion and explanation can be found in Istok [1989] and Kolditz [2002].

4.2.1.1.1 Discretising the problem domain

Elements are constructed from nodal points defined in space and joined by lines or arcs. The joined nodes can form 1, 2, or 3-Dimensional elements of varying shape e.g. triangles or quadrilaterals in 2D, and tetrahedra or hexahedra in 3D. The problem domain discretised into elements in this way is known as a mesh [Istok, 1989, Kolditz, 2002]. An example of finite element types is shown in Figure 4.2. Elements may be considered linear or quadratic depending on the number of nodes in the element. A linear element is one in which only the mesh node points are used for the integration of the approximated field variable and are suitable for hydraulic simulations, whereas a quadratic element contains additional nodal points at positions along the edges or faces of the element and are commonly used in mechanical solutions [Istok, 1989].

4.2.1.1.2 Discretising the governing equations

Once the problem domain is discretised into elements, the integral form of the governing partial differential equations are derived. The integral, or weak form is required in order to calculate situations where the solution may be discontinuous [Kolditz, 2002]. There are two main methods of discretising the equations into integral formulations known as variational principles/method, and the method of weighted residuals [Istok, 1989, Kolditz, 2002]. It is not always possible to find a variational principle for all problems so the method of weighted residuals, as implemented in OpenGeoSys, is most commonly used in hydraulic solutions [Istok, 1989, Kolditz et al., 2012, Kolditz, 2002].

The method of weighted residuals works by approximating the solution to the primary variable using shape functions specific to the element type chosen. This produces an error at each node known as the residual error which varies in magnitude and sign. All the residual errors from the connected elements and other nodes within the element are then weighted by shape functions, and this weighted average is forced to equal zero [Istok, 1989].

In order to illustrate the discretisation of Richards' equation in the finite element method Equation 4.7 is simplified by substituting Darcy's law and reducing to a one-dimensional case. Considering that hydraulic conductivity is related to permeability via:

$$K = \frac{\rho g}{\mu} k \quad (4.8)$$

and considering one-dimensional flow in the vertical direction, Equation 4.3 can be written to give the Darcy velocity ($\mathbf{q}$) as:

$$\mathbf{q} = -K_z(\psi) \frac{\partial \psi}{\partial z} \quad (4.9)$$

where ψ is the pressure head (m), and K_z denotes the hydraulic conductivity in the vertical axis. The storage function is converted from a saturation formulation to volumetric water content (θ). The relationship is:

$$\theta = nS \quad (4.10)$$

where S is the saturation, and n is the porosity. This is then used to define the specific moisture capacity:

$$C(\psi) = \frac{d\theta}{d\psi} \quad (4.11)$$

Following the assumption that the porosity is non-deformable [Thorenz, 2001], the storage term on the left hand side of Equation 4.7 can then be written as:

$$\left(S_{t_\alpha} S_\alpha n \frac{\partial S_\alpha}{\partial p_{c_\alpha}} \right) \frac{\partial p_{c_\alpha}}{\partial t} = C(\psi) \frac{\partial \psi}{\partial t} \quad (4.12)$$

where $C(\psi)$ is the specific moisture capacity. Thus, the one-dimensional simplified Richards equation in Darcy's law is:

$$\frac{\partial}{\partial z} \left[K_z(\psi) \left(\frac{\partial \psi}{\partial z} + 1 \right) \right] = C(\psi) \frac{\partial \psi}{\partial t} \quad (4.13)$$

where $K_z(\psi)$ is the hydraulic conductivity of the medium (m/s) as a function of pressure head (ψ) (m).

The Galerkin weighting function is commonly used in geoscience applications of the finite element method. In this method the weighting function used for the weighted average of residuals is the same as the shape functions used to approximate the value of the primary variable over the element [Istok, 1989]. Applying the Galerkin method of weighted residuals to the simplified unsaturated flow equation in 4.13 an approximate value of the pressure head ($\hat{\psi}^{(e)}$) is calculated as:

$$\hat{\psi}^{(e)} = \sum_{i=1}^n N_i^{(e)} \psi_i \quad (4.14)$$

where $N_i^{(e)}$ are the interpolation functions that are applied to the values of pressure head (ψ_i) at each node in the element e , and n is the number of nodes in the element [Istok, 1989]. When substituted back into the real solution this approximation causes an error at each node ($R_i^{(e)}$) given by:

$$R_i^{(e)} = - \int_{z_i^{(e)}}^{z_j^{(e)}} N_i^{(e)} \left[\frac{\partial}{\partial z} \left(K_z^{(e)}(\psi) \left(\frac{\partial \hat{\psi}}{\partial z} + 1 \right) \right) \right] dz + \int_{z_i^{(e)}}^{z_j^{(e)}} N_i^{(e)} C^{(e)}(\psi) \frac{\partial \hat{\psi}}{\partial t} dz \quad (4.15)$$

where $N_i^{(e)}$ are the weighting functions applied to the residual error, which in Galerkin's method are the same as the interpolation functions used to gain the approximate solution within the element. In this case a simple 1D scenario is discussed. Assuming that gravitational forces are negligible in comparison to capillary forces and that material properties are constant within an element but can change from element to element, the integral can be written as:

$$R_i^{(e)} = - \int_{z_i^{(e)}}^{z_j^{(e)}} N_i^{(e)} \left[K_z^{(e)}(\psi) \frac{\partial^2 \hat{\psi}}{\partial z^2} \right] + \int_{z_i^{(e)}}^{z_j^{(e)}} N_i^{(e)} C^{(e)}(\psi) \frac{\partial \hat{\psi}}{\partial t} dz \quad (4.16)$$

Applying the method of integration by parts to the first part of this equation gives:

$$\int_{z_i^{(e)}}^{z_j^{(e)}} N_i^{(e)} \left[K_z^{(e)}(\psi) \frac{\partial^2 \hat{\psi}^{(e)}}{\partial z^2} \right] dz = \left[N_i^{(e)} K_z^{(e)}(\psi) \frac{\partial \hat{\psi}^{(e)}}{\partial z} \right] - \int_{z_i^{(e)}}^{z_j^{(e)}} K_z^{(e)}(\psi) \frac{\partial N_i^{(e)}}{\partial z} \frac{\partial \hat{\psi}^{(e)}}{\partial z} dz \quad (4.17)$$

where the first expression on the right hand side describes the element flux across the element, and the second expression describes the distribution of the pressure head over the domain. Assuming the fluxes across the element will cancel out for all elements but boundary elements with specified Neumann boundary conditions, the first term can be neglected and the residual at node i described by:

$$R_i^{(e)} = - \int_{z_i^{(e)}}^{z_j^{(e)}} K_z^{(e)}(\psi) \frac{\partial N_i^{(e)}}{\partial z} \frac{\partial \hat{\psi}^{(e)}}{\partial z} dz \quad (4.18)$$

at node j the residual is:

$$R_j^{(e)} = - \int_{z_i^{(e)}}^{z_j^{(e)}} K_z^{(e)}(\psi) \frac{\partial N_j^{(e)}}{\partial z} \frac{\partial \hat{\psi}^{(e)}}{\partial z} dz \quad (4.19)$$

The approximated value ($\frac{\partial \hat{\psi}}{\partial z}$) can be re-written as:

$$\frac{\partial \hat{\psi}}{\partial z} = \frac{\partial N_i^{(e)}}{\partial z} \psi^{(e)} \quad (4.20)$$

Consequently, by separating the pressure head into a separate vector term, the matrix integral formulation for the conductance matrix $[K^{(e)}(\psi)]$ is derived directly from Equations 4.18

and 4.19 for this 1D two noded element as:

$$\left[K^{(e)}(\psi) \right] = \int_{z_i^{(e)}}^{z_j^{(e)}} \begin{bmatrix} K_z^{(e)}(\psi) \frac{\partial N_i^{(e)}}{\partial z} \frac{\partial N_i^{(e)}}{\partial z} & K_z^{(e)}(\psi) \frac{\partial N_i^{(e)}}{\partial z} \frac{\partial N_j^{(e)}}{\partial z} \\ K_z^{(e)}(\psi) \frac{\partial N_j^{(e)}}{\partial z} \frac{\partial N_i^{(e)}}{\partial z} & K_z^{(e)}(\psi) \frac{\partial N_j^{(e)}}{\partial z} \frac{\partial N_j^{(e)}}{\partial z} \end{bmatrix} dz \quad (4.21)$$

separating the constant $K_z^{(e)}(\psi)$ results in the expression for a general one dimensional element of length L with n number of nodes as:

$$\left[K^{(e)}(\psi) \right] = \int_L \begin{bmatrix} \frac{\partial N_1^{(e)}}{\partial z} \\ \vdots \\ \frac{\partial N_n^{(e)}}{\partial z} \end{bmatrix} \left[K_z^{(e)}(\psi) \right] \begin{bmatrix} \frac{\partial N_1^{(e)}}{\partial z} & \dots & \frac{\partial N_n^{(e)}}{\partial z} \end{bmatrix} dz \quad (4.22)$$

The element conductance matrices can now be written as:

$$\begin{Bmatrix} R_1^{(e)} \\ \vdots \\ R_n^{(e)} \end{Bmatrix}_K = \left[K^{(e)}(\psi) \right] \begin{Bmatrix} \psi_1 \\ \vdots \\ \psi_n \end{Bmatrix} \quad (4.23)$$

Evaluating the second term on the right hand side of equation 4.16 can be done in the same way to yield the element capacitance matrix [Istok, 1989]:

$$\begin{Bmatrix} R_1^{(e)} \\ \vdots \\ R_n^{(e)} \end{Bmatrix}_C = \left[C^{(e)}(\psi) \right] \begin{Bmatrix} \frac{\partial \psi_1}{\partial t} \\ \vdots \\ \frac{\partial \psi_n}{\partial t} \end{Bmatrix} \quad (4.24)$$

Two different forms of interpolation functions can be used to form the element capacitance matrix $[C^{(e)}(\psi)]$: a consistent formulation or a lumped formulation. Of the two, the lumped formulation provides the most numerically robust method because the consistent formulation can be susceptible to numerical oscillation [Istok, 1989, Kavetski et al., 2001, Rathfelder and Abriola, 1994]. In the consistent formulation the same interpolation function used to define $\hat{\psi}$ is used to define $\frac{\partial \psi}{\partial t}$, whereas the lumped formulation comprises a different function Istok [1989].

The lumped element formulation uses a different interpolation function (N^*) to define the time-derivative of the approximate solution [Istok, 1989]:

$$\left[C^{(e)}(\psi) \right] = \int_{L^{(e)}} \begin{bmatrix} N_1^{*(e)} \\ \vdots \\ N_n^{*(e)} \end{bmatrix} \left[C^{(e)}(\psi) \right] \begin{bmatrix} N_1^{*(e)} & \dots & N_n^{*(e)} \end{bmatrix} dz \quad (4.25)$$

These functions for a 1D bar element are such that:

$$N_i^* N_j^* = \begin{cases} \frac{1}{n} & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases} \quad (4.26)$$

where n is the number of nodes in the element. The capacitance matrix for a one dimensional element with 2 nodes ($n=2$), is therefore [Istok, 1989]:

$$\left[C^{(e)}(\psi) \right] = C^{(e)}(\psi) \frac{L^{(e)}}{n} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad (4.27)$$

4.2.1.1.3 Temporal discretisation of Richards' equation

Due to the time dependency of the capacitance matrix in equation 4.24, this system of equations must be discretised with respect to time as well as space. The most common method is the finite difference method. The vectors of pressure head and the derivative of pressure head with respect to time are redefined as:

$$\{\psi\} = \begin{Bmatrix} \psi_1 \\ \vdots \\ \psi_n \end{Bmatrix} \quad (4.28)$$

and:

$$\{\dot{\psi}\} = \begin{Bmatrix} \frac{\partial \psi_1}{\partial t} \\ \vdots \\ \frac{\partial \psi_n}{\partial t} \end{Bmatrix} \quad (4.29)$$

This results in the global finite element formulation being defined as:

$$\left[C(\psi) \right] \{\dot{\psi}\} + \left[K(\psi) \right] \{\psi\} = \{F\} \quad (4.30)$$

where $\{F\}$ is the flux vector containing any specified Neumann boundary conditions. The finite difference method can be applied to this equation to determine the value of ψ and $\frac{\partial \psi}{\partial t}$ over the model domain.

A value of the primary variable may be determined at any point in time by applying the mean value theorem of calculus. The time derivative of ψ at any point (ξ) between a time interval Δt can be found from the difference between the value of ψ at either end of the time interval:

$$\frac{\partial \psi}{\partial t}(\xi) = \frac{\psi_{t+\Delta t} - \psi_t}{\Delta t} \quad (4.31)$$

This is shown graphically in Figure 4.3. The value of ψ at point ξ can be defined as:

$$\psi(\xi) = \psi(t) - (\xi - t) \frac{\partial \psi}{\partial t}(\xi) \quad (4.32)$$

The exact position of the point between the time intervals is unknown and there are a number of different approaches of the finite difference scheme to solve for different locations along the time interval. To determine the location of ξ along the time interval a variable (ω) is defined:

$$\omega = \frac{\xi - t}{\Delta t} \quad (4.33)$$

This is then used to essentially weight the contributions of ψ from either end of the time interval, for example:

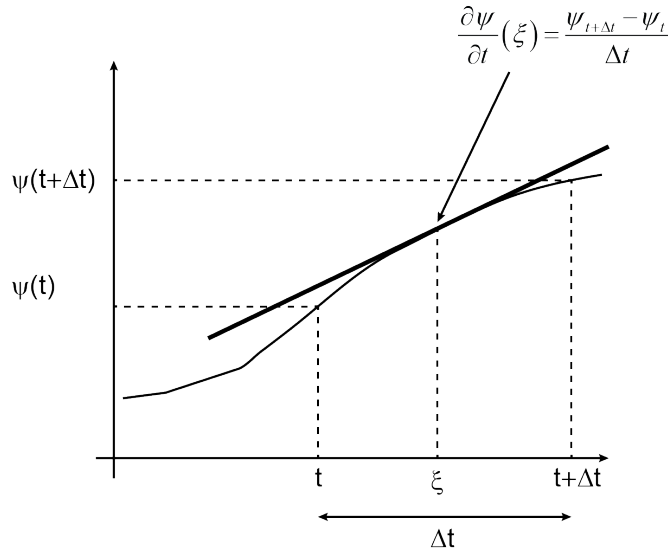


Figure 4.3: A graphical representation after Istok [1989] illustrating the calculation of the time derivative of the primary variable at any point in the time interval.

$$\psi(\xi) = (1 - \omega)\psi(t) + \omega\psi(t + \Delta t) \quad (4.34)$$

This can be used in the pressure head and flux vectors of the finite element formulation:

$$\{\psi\} = (1 - \omega) \{\psi\}_t + \omega \{\psi\}_{t+\Delta t} \quad (4.35)$$

$$\{F\} = (1 - \omega) \{F\}_t + \omega \{F\}_{t+\Delta t} \quad (4.36)$$

Incorporating these equations into the finite element formulation of equation 4.30 leads to the finite difference formulation of the transient unsaturated flow equation:

$$([C(\psi)] + \omega\Delta t [K(\psi)]) \{\psi\}_{t+\Delta t} = ([C(\psi)] - (1 - \omega)\Delta t [K(\psi)]) \{\psi\}_t + \Delta t ((1 - \omega)\{F\}_t + \omega\{F\}_{t+\Delta t}) \quad (4.37)$$

The choice of the value ω will define the type of finite difference method used:

- $\omega = 0.0$ uses the known values at t and is known as the Forward Difference Method,
- $\omega = 0.5$ uses the value half way between the time interval and is known as the Central Difference Method, and
- $\omega = 1.0$ uses the value at $t + \Delta t$ and is known as the Backward Difference Method.

In unsaturated fluid flow simulations using the Richard equation the Backwards Difference Method is most commonly employed.

4.2.1.1.4 Developing a system of equations

The method of weighted residuals produces a system of matrix-integral expressions describing the distribution of the field variable across the model domain [Istok, 1989]. Interpolation

functions were used to approximate the value of the field variable across each element and are therefore specific to the shape of each element. For simple linear elements, such as the 1D bar element or linear triangle, an analytical solution is sufficient to determine the interpolation functions for each element [Istok, 1989]. However, for more complex elements and large meshes, determining individual interpolation functions for each element is a laborious process. Transforming the global coordinates of each element to local coordinates of a reference element allows the definition of integration points within the reference element, known as Gauss points, each with their own constant interpolation functions to the nodes. This greatly simplifies the integration procedure [Istok, 1989].

In Equation 4.18 and 4.19 the interpolation functions are defined in terms of the global nodal coordinates (in this case the z axis). Transforming the element to a reference element defined in a local coordinate system allows the same local interpolation functions to be used for every element. Global interpolation functions are given by [Istok, 1989] as a function of the global coordinate system:

$$\left[\frac{\partial N_i^{(e)}}{\partial z} \quad \dots \quad \frac{\partial N_n^{(e)}}{\partial z} \right] \quad (4.38)$$

The coordinate transformation takes the form:

$$x = f(\xi) \quad (4.39)$$

where ξ is the local coordinate system [Istok, 1989]. Rewriting the interpolation functions in terms of these local coordinates gives:

$$\frac{\partial N_i^{(e)}}{\partial z} = \frac{\partial N_i^{(e)}}{\partial \xi} \frac{\partial \xi}{\partial z} = \frac{\partial N_i^{(e)}}{\partial \xi} [J] \quad (4.40)$$

where $[J]$ is the Jacobian transformation matrix [Istok, 1989]. The inverse of the transformation matrix converts the local coordinate interpolation functions into global coordinates. Using this transformation procedure the matrix integral in Equation 4.41 can be re-written for the numerical integration as:

$$[K^{(e)}] = \int_{L_\xi} \begin{bmatrix} \frac{\partial N_1^{(e)}}{\partial \xi} \\ \vdots \\ \frac{\partial N_n^{(e)}}{\partial \xi} \end{bmatrix} [J^{-1}]^T [K_z^{(e)}] [J^{-1}] \begin{bmatrix} \frac{\partial N_1^{(e)}}{\partial \xi} & \dots & \frac{\partial N_n^{(e)}}{\partial \xi} \end{bmatrix} |J| d\xi \quad (4.41)$$

where $|J|$ is the determinant of the Jacobian matrix.

The capacitance matrix uses different interpolation functions in the lumped formulation and becomes:

$$[C^{(e)}(\psi)] = C^{(e)}(\psi) \frac{L^{(e)}}{n} |J| \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad (4.42)$$

Combining the element conductance matrices and element capacitance matrices into global conductance and global capacitance matrices leads to the finite element formulation for transient unsaturated fluid flow:

$$[C(\psi)] \begin{Bmatrix} \frac{\partial \psi_1}{\partial t} \\ \vdots \\ \frac{\partial \psi_n}{\partial t} \end{Bmatrix} + [K(\psi)] \begin{Bmatrix} \psi_1 \\ \vdots \\ \psi_n \end{Bmatrix} = \{F\} \quad (4.43)$$

Alternative terminology for the two main portions of this equation can be used. The conductance matrix can also be termed the Laplace matrix, and the capacitance matrix is also known as the Mass matrix. Boundary conditions are applied as known values of pressure in the pressure vector, and source terms are incorporated in the flux vector. The boundary conditions are calculated through the system of equations eliminating the boundary nodes and reducing the size of the global capacitance and conductance matrices. The non-linear nature of Richards' equation requires the use of an iterative solution procedure such as a Picard or Newton-Rapheson iteration. Istok [1989] neatly explains these methods.

4.3 Hydraulic Model - Developments

The key developments in the hydraulic model include the implementation of Dueck suction as a means to define the stress-dependent water retention curve, the conversion of water content to saturation in order to use the experimentally derived free swell water retention data, and the implementation of a variety of permeability models (presented in Chapter 3).

4.3.1 Water Retention Curve

The water retention curve has been shown to be an increasingly important requirement for constitutive modelling of unsaturated soils [Fredlund et al., 2012, Fredlund and Xing, 1994]. In Richards' equation the water retention curve provides the constitutive relationship between the degree of saturation and the suction pressure that is required to close the non-linear equation. Models for the water retention curve (or soil-water characteristic curve) are introduced in Chapter 3 with two main fields of model identified:

- those based upon fitting a constant volume water retention curve and then extrapolated to changes in volume e.g. Gallipoli et al. [2003], and
- those concerned with addressing the water retention behaviour under free swell conditions and adjusting for varying degrees of confinement based on the mechanical stress [Dueck and Börgesson, 2007].

In this work the modelling application of the SEALEX experiments involves hydro-mechanical conditions from constant volume to free swell during Step 2 and Step 3 and therefore the second approach to modelling the water retention curve is employed. The free swell water retention data are fitted with an empirical function from Bond and Benbow [2009]:

$$s_{fs} = M_b(\exp(a - bM_w) + \exp(c - dM_w)) \quad (4.44)$$

where s_{fs} is the free swell suction, M_w is the gravimetric water content, M_b is the mass fraction of bentonite in the mixture, and a, b, c , and d are all fitting constants. The empirical fit provides a smooth curve for the relationship between gravimetric water content and suction which is then related to the confining stress via the Dueck suction concept. As discussed in

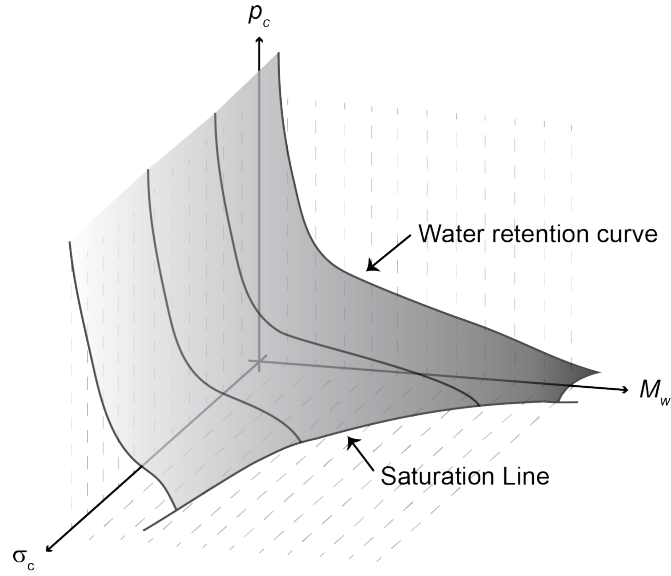


Figure 4.4: A schematic diagram of the constitutive state surface for the water retention properties of bentonite between suction (denoted as p_c in this figure), gravimetric water content, and confining stress.

Chapter 3, this method describes a constitutive state surface linking the suction (s), gravimetric water content (M_w), and confining stress (σ_c), which is applicable for conditions of constant volume to free-swell and up to confining stresses equal to the swelling pressure. A schematic diagram of this state surface is presented in Figure 4.4 and each individual relationship between the three variables is interpreted as;

- In the plane of $s - M_w$ the water retention curve defines a point of maximum water content for a given suction at zero stress.
- In the plane of $M_w - \sigma_c$ the surface defines the maximum water content for a range of swelling pressures at a given suction i.e. a line defining saturation.
- In the plane of $\sigma_c - s$ the surface is constant because at a given water content there can be no change in suction with a change in confining stress- in order for a change in suction to occur there must be a change in water content.

The state surface shown in Figure 4.4 describes the upper bounds of water contents for a given initial void ratio or dry density and represents a link between the hydraulic and mechanical processes through the concept of Dueck suction [Dueck and Börgesson, 2007]. The maximum water content ($M_{w_{max}}$) at a given void ratio is a function of the available porosity and is calculated from:

$$M_{w_{max}} = \frac{n}{\left(\frac{\rho_d}{\rho_{ref}}\right)} \quad (4.45)$$

where n is the porosity, ρ_d is the dry density of the sample (kg/m^3), and ρ_{ref} is a reference density, which in this case is that of freshwater: $1000 \text{ kg}/\text{m}^3$. The porosity of a sample is determined from the dry density as:

$$n = 1 - \frac{\rho_d}{\rho_s} \quad (4.46)$$

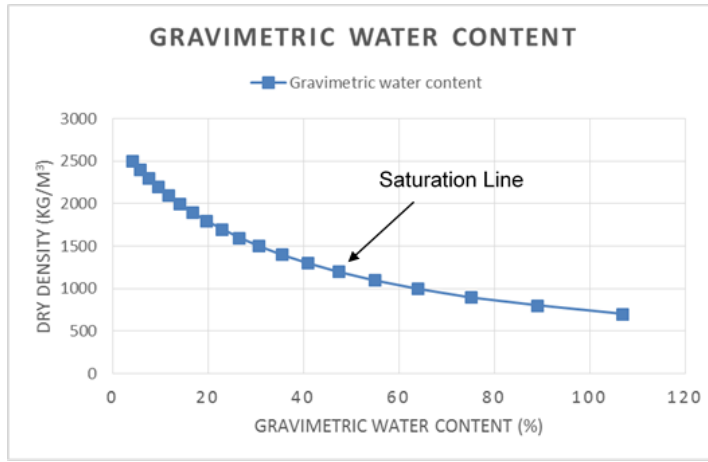


Figure 4.5: A graph of the maximum water content of a sample in relation to the dry density indicating the saturation line.

where ρ_s is the density of the solids. Consequently, the size and position of the state surface presented in Figure 4.4 must therefore be a function of the dry density of the sample for stress conditions that cause a reduction in void ratio below the initial conditions. A graph showing the effect of dry density on the gravimetric water content is shown in Figure 4.5 and highlights the logical relationship that at high dry densities the water content is reduced. The effect of this is to shift the saturation line shown in Figure 4.4 left along the gravimetric water content axis thereby reducing the maximum water content in the $\sigma_c - M_w$ plane.

During isotropic consolidation test conditions the void ratio is reduced below that of the initial conditions. Failure to take into account the change in maximum water content at void ratios below initial conditions results in a fully reversible water content behaviour for a loading-unloading stress path [Gallipoli et al., 2003]. For samples that exhibit unrecoverable strains this leads to erroneous calculations of saturation because the permanent change in void ratio is not incorporated into the hydraulic solution. In order to overcome this issue and account for changes to the saturation of a sample during isotropic loading-unloading stress paths, the maximum water content for a given dry density is used to update the location of the saturation line. The methodology for this is discussed later in this section.

4.3.1.1 Converting gravimetric water content to saturation

The water retention curve is experimentally determined as a relationship between the gravimetric water content and the total suction. Equation 4.7 defines the water retention curve in terms of saturation and total suction, and this is the in-built relationship in OpenGeoSys. Typically the water retention curve is defined by the van Genuchten [van Genuchten, 1980] or the Brooks and Corey [Brooks and Corey, 1964] functions which are formulated with respect to degree of saturation. Therefore, in order to incorporate the experimentally derived relationship between gravimetric water content and suction within the current Richards equation framework, the gravimetric water content was converted to a saturation. Saturation enters Richards' equation in the storativity term in Equation 4.7:

$$\left(S_{t\alpha} S_\alpha + n \frac{\partial S_\alpha}{\partial p_{c\alpha}} \right) \quad (4.47)$$

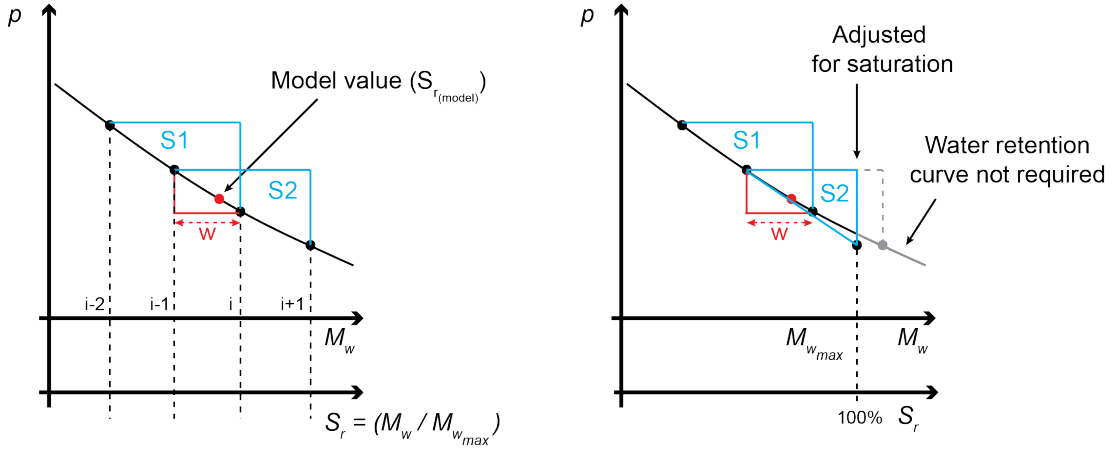


Figure 4.6: Schematic diagrams to show the method of calculating $\frac{\partial p_{c\alpha}}{\partial S_\alpha}$ from the gravimetric water content-suction experimentally derived relationship. The model value of saturation is scaled to a saturation by the maximum water content. S1 and S2 represent the gradient of the relationship across three points straddling the model value of saturation (Equations 4.49 and 4.50), and w is the weighting function between the two gradients (Equation 4.51). If the conversion of water content to saturation results in one of the points exceeding 100% saturation the water retention curve is limited to 100% saturation and the gradient adjusted.

In both instances the saturation is determined from:

$$S_\alpha = \frac{M_w}{M_{w_{max}}} \quad (4.48)$$

However, using the water content - suction experimental relationship requires the currently implemented calculation of the derivative of the saturation with respect to suction in OpenGeoSys to be updated to read in water content. Figure 4.6 shows the calculation method to determine the derivative of suction pressure with respect to saturation from the experimental results of the suction pressure - gravimetric water content relationship.

Currently the derivative of saturation is calculated from the gradient of the experimental data calculated across three increments of water content straddling the model value and scaled by a weighting function (Figure 4.6). The phase subscript is dropped for the following description of the calculation of the derivative of suction with respect to saturation to avoid confusion with the location of the calculation points in Figure 4.6:

$$S1 = \frac{dp}{dS} = \frac{0.5p_i - 0.5p_{i-2}}{0.5S_i - 0.5S_{i-2}} \quad (4.49)$$

$$S2 = \frac{dp}{dS} = \frac{0.5p_{i+1} - 0.5p_{i-1}}{0.5S_{i+1} - 0.5S_{i-1}} \quad (4.50)$$

$$w = \frac{S_m - S_{i-1}}{S_i - S_{i-1}} \quad (4.51)$$

where notation is that shown in Figure 4.6. The derivative of suction with respect to saturation is then given by:

$$\frac{\partial p}{\partial S} = (1 - w)S1 + wS2 \quad (4.52)$$

Richards' equation requires the derivative of saturation with respect to suction pressure and so the inverse of Equation 4.52 is calculated:

$$\frac{\partial S}{\partial p} = \left((1-w)S1 + wS2 \right)^{-1} \quad (4.53)$$

As the experimental gravimetric water content - suction relationship is read into the code, the saturation values in the above equations are scaled from the water contents i.e.:

$$S1 = \frac{0.5p_i - 0.5p_{i-2}}{0.5\left(\frac{M_w}{M_{wmax}}\right)_i - 0.5\left(\frac{M_w}{M_{wmax}}\right)_{i-2}} \quad (4.54)$$

$$S2 = \frac{0.5p_{i+1} - 0.5p_{i-1}}{0.5\left(\frac{M_w}{M_{wmax}}\right)_{i+1} - 0.5\left(\frac{M_w}{M_{wmax}}\right)_{i-1}} \quad (4.55)$$

$$w = \frac{\left(\frac{M_w}{M_{wmax}}\right)_m - \left(\frac{M_w}{M_{wmax}}\right)_{i-1}}{\left(\frac{M_w}{M_{wmax}}\right)_i - \left(\frac{M_w}{M_{wmax}}\right)_{i-1}} \quad (4.56)$$

In the instance when a sample nears saturation and the value of $i+1$ exceeds 1.0 (saturation) then this value is scaled back to 1.0 along the water content axis. The effect of this is to limit the water retention curve to 100% saturation. The 100% saturation point is dependent on the volume of the sample and can vary throughout the solution depending on the mechanical solution. This essentially moves along the water content axis depending on the deformation.

4.3.2 Permeability Model

4.3.2.1 Intrinsic permeability

There are a number of permeability models that have been proposed for the modelling of bentonite and these are introduced in Chapter 3. Of these, a variety of permeability models have been implemented and tested, including:

- Constant permeability
- The in-built Kozeny-Carmen equation
- An empirical permeability model after Karnland et al. [2006], and
- The KC-like equation proposed by Liu et al. [2011].

4.3.2.2 Relative permeability

The relative permeability model implemented is simply the power law function suggested by Brooks and Corey [1964].

$$k_{rel} = S^\eta \quad (4.57)$$

where S is the saturation, and η is the exponent.

4.4 Mechanical Model - Theory

The mechanical model framework employed in this work is that of non-linear elasticity. A new Young's modulus (E) is calculated at the end of each step using the formula proposed later in this section, and updated for each element as a function of the strain. Therefore an explicit assumption is made whereby the strain calculated from the previous solution informs the non-linear material properties for the subsequent time-step. In this section a finite element formulation for linear elasticity is presented after Lewis and Schrefler [1998] before the developed non-linear elastic model is proposed.

In continuum mechanics three unknown fields are the object of the calculation; displacements, stresses, and strains. These are independent of the material investigated but linked through constitutive relationships that are specific to the material e.g. Hooke's law of linear elasticity.

Stress is defined as force per unit area and is represented by the second-order tensor:

$$\boldsymbol{\sigma} = \begin{bmatrix} \sigma_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \sigma_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \sigma_{zz} \end{bmatrix} \quad (4.58)$$

where σ is the stress in the cartesian coordinate axes and τ is shear stress. Strains are represented by the strain tensor as:

$$\boldsymbol{\epsilon} = \begin{bmatrix} \epsilon_{xx} & \gamma_{xy} & \gamma_{xz} \\ \gamma_{yx} & \epsilon_{yy} & \gamma_{yz} \\ \gamma_{zx} & \gamma_{zy} & \epsilon_{zz} \end{bmatrix} \quad (4.59)$$

where ϵ is strain in the cartesian coordinate axes and γ is shear strain. Volumetric strain is the summation of the strain in each cartesian axis.

Strain is related to the displacement (u) through the symmetric gradient operator (often denoted as L) by:

$$\boldsymbol{\epsilon} = L\mathbf{u} \quad (4.60)$$

where L is given by (in 3D);

$$L = \begin{bmatrix} \frac{\partial}{\partial x} & 0 & 0 \\ 0 & \frac{\partial}{\partial y} & 0 \\ 0 & 0 & \frac{\partial}{\partial z} \\ \frac{\partial}{\partial y} & \frac{\partial}{\partial x} & 0 \\ 0 & \frac{\partial}{\partial z} & \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} & 0 & \frac{\partial}{\partial x} \end{bmatrix} \quad (4.61)$$

Stress and strain are linked via a constitutive relationship that considers the material parameters of the sample in question. For linear elasticity this constitutive relationship is defined by the generalized Hooke's Law:

$$\boldsymbol{\sigma} = \mathbf{E}\boldsymbol{\epsilon} \quad (4.62)$$

where σ is the stress, E is the Young's modulus (Pa), and ϵ is the volumetric strain (-). This can be extended to non-linear elasticity by considering an update to the material parameters (E) through the solution e.g. as a function of strain.

4.4.1 Finite Element Formulation of Linear Elasticity

The finite element formulation takes the form:

$$\mathbf{K}\mathbf{u} = \mathbf{f} \quad (4.63)$$

where $\mathbf{K}$ is the stiffness matrix containing the material parameters, $\mathbf{u}$ is the displacement vector of known and unknown displacements, and $\mathbf{f}$ is the force vector containing the body forces and any specified traction forces i.e. applied loads on the surface of the system.

The stiffness matrix is calculated on an element by element basis as a function of the material parameters and the element interpolation functions. The interpolation functions are specific to each element shape and interpolate the displacement field over the element:

$$\mathbf{u}(x, y, z) = \begin{bmatrix} u_x(x, y, z) \\ u_y(x, y, z) \\ u_z(x, y, z) \end{bmatrix} = \begin{bmatrix} N_1^{(e)} & 0 & 0 & \dots & N_n^{(e)} & 0 & 0 \\ 0 & N_1^{(e)} & 0 & \dots & 0 & N_n^{(e)} & 0 \\ 0 & 0 & N_1^{(e)} & \dots & 0 & 0 & N_n^{(e)} \end{bmatrix} \mathbf{u}^{(e)}(x, y, z) \quad (4.64)$$

Recalling that the strain is related to the displacement through the symmetric gradient operator, the interpolated strain at each node in a 3-D element is given by:

$$\epsilon(x, y, z) = \begin{bmatrix} \frac{\partial N_1^{(e)}}{\partial x} & 0 & 0 & \dots & \frac{\partial N_n^{(e)}}{\partial x} & 0 & 0 \\ 0 & \frac{\partial N_1^{(e)}}{\partial y} & 0 & \dots & 0 & \frac{\partial N_n^{(e)}}{\partial y} & 0 \\ 0 & 0 & \frac{\partial N_1^{(e)}}{\partial z} & \dots & 0 & 0 & \frac{\partial N_n^{(e)}}{\partial z} \\ \frac{\partial N_1^{(e)}}{\partial y} & \frac{\partial N_1^{(e)}}{\partial x} & 0 & \dots & \frac{\partial N_n^{(e)}}{\partial y} & \frac{\partial N_n^{(e)}}{\partial x} & 0 \\ 0 & \frac{\partial N_1^{(e)}}{\partial z} & \frac{\partial N_1^{(e)}}{\partial y} & \dots & 0 & \frac{\partial N_n^{(e)}}{\partial z} & \frac{\partial N_n^{(e)}}{\partial y} \\ \frac{\partial N_1^{(e)}}{\partial z} & 0 & \frac{\partial N_1^{(e)}}{\partial x} & \dots & \frac{\partial N_n^{(e)}}{\partial z} & 0 & \frac{\partial N_n^{(e)}}{\partial x} \end{bmatrix} \mathbf{u}^{(e)}(x, y, z) = \mathbf{L}N^{(e)}\mathbf{u}^{(e)}(x, y, z) \quad (4.65)$$

The matrix $\mathbf{L}N$ is often denoted as $\mathbf{B}$ and is referred to as the strain-displacement matrix. Matrix $\mathbf{B}$ calculates how the displacement vector is interpolated across the element to give the strain. However, displacements are the result of a change in stress and therefore matrix $\mathbf{B}$ can only describe the material behaviour with a constitutive relationship between stress and strain e.g. elasticity.

The material elastic properties are described by the elastic constitutive matrix ($\mathbf{D}^{(e)}$):

$$\mathbf{D}^{(e)} = \frac{E}{(1 + \nu)(1 - 2\nu)} \begin{bmatrix} 1 - \nu & \nu & \nu & 0 & 0 & 0 \\ \nu & 1 - \nu & \nu & 0 & 0 & 0 \\ \nu & \nu & 1 - \nu & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1-2\nu}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1-2\nu}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1-2\nu}{2} \end{bmatrix} \quad (4.66)$$

where E is the Young's modulus (Pa), and ν is the Poisson's Ratio (-).

The stiffness matrix that is used in Equation 4.63 to determine displacements from a change in stress is then built from:

$$\mathbf{K}^{(e)} = \int_{\Omega^{(e)}} h \mathbf{B}^T \mathbf{D} \mathbf{B} d\Omega^{(e)} \quad (4.67)$$

where h is the element thickness (in 2D this is unit thickness), the superscript T refers to the transpose of the matrix, and $\Omega^{(e)}$ is the element area. The force vector contains any internal body forces ($\mathbf{b}$) and any surface tractions ($\hat{\mathbf{t}}$) and can be expressed as:

$$\mathbf{f}^{(e)} = \int_{\Omega^{(e)}} h \mathbf{N}^T \mathbf{b} \Omega^{(e)} + \int_{\Gamma^{(e)}} h \mathbf{N}^T \hat{\mathbf{t}} d\Gamma^{(e)} \quad (4.68)$$

where $\Gamma^{(e)}$ is the element boundary to which a surface traction ($\hat{\mathbf{t}}$) may be applied. Each element stiffness matrix and force vector is combined to form the global system of equations that can be solved to determine nodal displacements by inverting the stiffness matrix:

$$\mathbf{u} = \mathbf{K}^{-1} \mathbf{f} \quad (4.69)$$

Boundary conditions can be specified as a given value of displacement in the displacement vector or as a traction force in the force vector.

4.5 Mechanical Model - Developments

The main development of the mechanical model is the implementation of a strain depend non-linear elastic model. The implementation of the non-linear elastic function is closely linked to the development of the moving mesh, which is discussed separately in Section 4.7.

4.5.1 The Non-Linear Elastic model developed in this thesis

A non-linear elastic mechanical model based on the strain history of the sample is developed to describe the mechanical behaviour of bentonite under varying stress conditions e.g. constant volume, free swell, and consolidation. An explicit assumption for the material properties is used such that Hooke's Law is calculated for each timestep but non-linearity is achieved by updating the Young's modulus as a function of the strain on the sample. Hooke's law is:

$$\sigma = E \epsilon \quad (4.70)$$

where σ is the stress, E is the non-linear Young's modulus (Pa), and ϵ is the volumetric strain (-). The Young's modulus is updated at each time-step and is given by the following strain dependent empirical formula adapted from that developed by Bond et al. [2014] for the initial stages of DECOVALEX-2015:

$$E_t^{(e)} = E_{t=0}^{(e)} \left(1 + \left(\alpha \sum_{t=1}^{t-1} \Delta \epsilon_{v_t}^{(e)} \right)^d \right) \quad (4.71)$$

where $E_t^{(e)}$ (Pa) is the updated Young's modulus for the given time-step t at element e , $E_{t=0}^{(e)}$ is the initial Young's modulus or reference stiffness (Pa), α is the hardening or softening factor

depending on the strain direction (α_h and α_s respectively), $\sum_{t=1}^t \Delta\epsilon_{v_t}^{(e)}$ is the total volumetric strain the element has seen up to time t , and d is a fitting parameter know as the dimension.

This function leads to an increase in elastic modulus with a decrease in sample volume i.e. consolidation hardening, and also a decrease in elastic modulus with an increase in sample volume i.e. expansion softening. The initial void ratio of the sample is used as a control to switch between the softening and hardening factors in the calculation of the Young's modulus. This allows softening and hardening parameters that reflect the different stress states and strain directions to be defined separately. As a result four different conditions are considered:

- volume reduction at void ratios greater than the initial void ratio,
- volume expansion at void ratios greater than the initial void ratio,
- volume reduction for void ratios less than the initial value, and
- volume expansion for void ratios less than the initial value.

For the first two cases the hardening and softening parameters are equal to the user defined softening parameter. For the third case the hardening parameter takes the user defined value, and for the final case linear elastic rebound is assumed by calculating a constant Young's modulus.

The non-linear elasticity function proposed in Equation 5.10 is developed with a Lagrangian moving mesh (as described in the next section). The increment of element strain for each time-step is calculated from:

$$\Delta\epsilon_{v_t}^{(e)} = \frac{V_t^{(e)} - V_{t-1}^{(e)}}{V_{t-1}^{(e)}} \quad (4.72)$$

where the V_{t-1} refers to the element volume at the end of the last time interval, V_t is the calculated element volume in the current time interval, and $\Delta\epsilon_{v_t}^{(e)}$ is the increment of strain of the element. The total volumetric strain of the element at time t is calculated from:

$$\epsilon_{v_t}^{(e)} = \Delta\epsilon_{v_t}^{(e)} + \left(\sum_{t=1}^{t-1} \Delta\epsilon_{v_t}^{(e)} (1 + \Delta\epsilon_{v_t}^{(e)}) \right) \quad (4.73)$$

The increment of volumetric strain is used to determine a new element void ratio ($\eta^{(e)}$) as:

$$\eta_t^{(e)} = \eta_{t-1}^{(e)} + \left(\Delta\epsilon_{v_t}^{(e)} (1 + \eta_{t-1}^{(e)}) \right) \quad (4.74)$$

Here void ratio is given the symbol η to avoid confusion with the element notation (e). A new element porosity ($n^{(e)}$) is determined from the void ratio:

$$n^{(e)} = \frac{\eta^{(e)}}{1 + \eta^{(e)}} \quad (4.75)$$

Element dry density ($\rho_d^{(e)}$) is updated as a function of the change in element volume:

$$\rho_d^{(e)} = \frac{m_{s(t=0)}^{(e)}}{V_t^{(e)}} \quad (4.76)$$

where $m_{s(t=0)}$ is the mass of the solids in the starting material (kg).

This empirical formula was developed in line with the experimental consolidation tests and therefore requires extension to account for stress conditions that permit large expansive strains in order to ensure that the Young's modulus is not able to be ≤ 0 :

$$E_t^{(e)} = \left(E_{min} \sum_{t=1}^{t-1} \Delta \epsilon_{v_t}^{(e)} \right) \exp^{k_{red}} \quad (4.77)$$

where E_{min} is a user defined Young's modulus threshold below which the effect of strain on reducing Young's modulus is reduced, and k_{red} is a negative exponent that controls the rate of reduction of Young's modulus with continued strain. This extension only applies in expansion and when the calculated Young's modulus is below a defined threshold. The Young's modulus used in the simulation step is then:

$$E_t^{(e)} = \begin{cases} E_{t=0}^{(e)} \left(1 + \left(\alpha \sum_{t=1}^{t-1} \Delta \epsilon_{v_t}^{(e)} \right)^d \right) & \text{for } E_t^{(e)} > E_{min} \\ \left(E_{min} \sum_{t=1}^{t-1} \Delta \epsilon_{v_t}^{(e)} \right) \exp^{k_{red}} & \text{for } E_t^{(e)} < E_{min} \end{cases} \quad (4.78)$$

As water content is closely linked to expansive strains in free swell conditions this function implies that at higher suctions a small change in water content has a larger effect on the mechanical material properties than at low suctions. This aims to reflect the transition from dry, stiff conditions towards a gel so that, at low suctions and large strains further expansion occurs with a less pronounced change in mechanical material parameters.

4.6 Hydro-Mechanical Coupling

The saturation and subsequent build of stress or volume change of bentonite is an extremely strongly coupled Hydro-Mechanical process (HM). The conceptual understanding of the process suggests that it is primarily driven by the alleviation of suction pressure as the sample hydrates i.e. as the water enters the sample it either increases in volume to accommodate this extra fluid, or a pressure/stress begins to build up on the constraining material as the sample tries to increase in volume but cannot [Agus et al., 2012, Baille et al., 2010, Gens and Alonso, 1992, Komine and Ogata, 1996]. Consequently the HM coupling approach aims to reflect this underlying process by linking the change in suction to a change in stress in the mechanical formulation. This section describes the coupling procedure for the hydraulic and mechanical processes in both directions by addressing the stress conditions and the staggered HM coupling scheme.

Coupling is achieved via the Dueck suction concept which states that the net suction (s_{net}) within a sample is a function of the free swell suction (s_{fs}) and the applied external stress (σ_c) (Equation 3.34 is repeated here for ease) [Dueck, 2004, Dueck and Börjesson, 2007]:

$$s_{net} = s_{fs} - \sigma_c \quad (4.79)$$

This assumption results in the hydraulic primary variable, suction pressure, being a function of the stress state of the sample:

$$s = f(\sigma_c) \quad (4.80)$$

where s is the suction pressure (Pa), and σ_c is the confining stress (Pa). As discussed in Chapter 3, the Dueck suction concept is also fundamental to the description of the water retention behaviour. This provides a direct coupling between the two processes and ensures that the energy required to change the saturation is linked to the total stress state of the soil.

This concept gives rise to three variables that describe the hydraulic and mechanical stress states; confining stress, net suction, and free swell suction. The relationship of these variables is given by Equation 4.79. Richards' equation incorporates the stress dependent water retention curve and calculates a solution for the suction pressure as a function of the stress. It therefore calculates net suction as a result of the stress dependency of the water retention properties. This becomes an important consideration when the sample undergoes a reversal in stress conditions e.g. from consolidation to unloading, or constant volume conditions to loss of confinement. As net suction is a function of the stress state and the free swell suction, if the stress conditions change abruptly e.g. with loss of confinement, the net suction changes. This dependency of the hydraulic potential on the mechanical stress can be thought of as an M-H coupling, which needs to be considered when defining the input for Richards' flow equation to ensure net suction is the primary variable.

Similarly, if confining stress has a direct link with the suction pressure, the suction pressure therefore provides a hydraulic stress that must be considered in the calculation of the mechanical solution. For example, when there is no confinement the alleviation of suction will produce a stress that leads to a change in volume of the sample. Therefore, the change in suction is equivalent to an elastic mechanical source term, which can be considered to be coupling in the H-M direction.

Consequently total effective stress can be defined as:

$$\sigma_T = \sigma_M + \sigma_H \quad (4.81)$$

where the subscripts T , M , and H refer to the total, mechanical, and hydraulic stresses respectively. The hydraulic stress is a function of the free swell suction change and is calculated from the change in water content determined by the hydraulic solution.

4.6.1 Effective stresses

The definition of stress in Equation 4.81 is, in essence, similar to the effective stress principle discussed in Chapter 3 and defined as:

$$\sigma' = p + s \quad (4.82)$$

where σ' is the effective stress, and p is the net mean stress. s is the total suction, which is a negative value i.e. less than atmospheric pressure. The mechanical stress in Equation 4.81 is the net mean stress (p) defined as:

$$p = \frac{1}{3}(\sigma_x + \sigma_y + \sigma_z) \quad (4.83)$$

where the subscripts x , y , and z refer to the cartesian axes.

In the effective stress definition, typically the hydraulic stress is defined in terms of the matric suction. The Bishop effective stress is commonly used in constitutive modelling of unsaturated soils because it combines information of the suction and saturation states of the

soil [Gens et al., 2006]:

$$\sigma' = (\sigma - u_a) + \chi(u_a - u_w) \quad (4.84)$$

where χ is Bishop's parameter that has been shown to correspond closely to saturation [Gens et al., 2006, Lewis and Schrefler, 1998], and u_a and u_w are the pore air pressure and pore water pressure respectively that are used to define the matric suction [Lewis and Schrefler, 1998]. However, as bentonite has been shown to have only a small contribution of matric suction [Agus et al., 2010], σ_H in Equation 4.81 refers to the total suction as defined by the water retention properties. As the total suction corresponds to the suction pressure defined previously in the hydraulic model as p_c , this definition of suction pressure is used here:

$$\sigma' = (\sigma - u_a) + \mathbf{I}(\chi s) \quad (4.85)$$

where $\mathbf{I}$ is the identity matrix and ensures that the effect of the fluid pressure is purely volumetric.

4.6.1.1 Internal Strain Factor

Equation 4.84 calculates the effective stress considering a non-deformable pore space. However, the hydration process of montmorillonite results in a constantly evolving pore space as aggregates expand and, in some cases, exfoliate to cause new pore sizes and clog other pore sizes [Likos and Lu, 2006, Pusch et al., 1990, Wang, 2012, Wayllace, 2008]. At low water contents a reduction in suction causes swelling of clay clusters that is initially accommodated by crystalline swelling of aggregates into the macro-void spaces [Likos and Lu, 2006, Wayllace, 2008]. As a result only a small portion of the suction change is translated to the skeleton as a change in effective stress. However, at higher water contents the bentonite clusters have expanded to fill the macro-void spaces (under constant volume conditions) and the majority of further suction change corresponds to a mechanical stress acting on the skeleton. If the sample is unconstrained then the bulk volume change for a given change in suction at low water contents is comparatively low as the macro-voids are filled by the expanding bentonite, but at higher water contents a given change in suction produces a much greater change in volume [Likos and Lu, 2006]. This is in part because the water adsorption mechanisms transition from crystalline swelling, that is dominant from high suction to around 20 MPa suction, to osmotic swelling which is dominant <0.8 MPa suction [Wayllace, 2008]. Typically for expansive clays, it is assumed that the intra-aggregate porosity is fully saturated i.e. crystalline swelling is complete, before osmotic swelling predominates at water contents of >40 % [Madsen and Müller-Vonmoos, 1989, Wayllace, 2008].

In order to represent both the accommodation of aggregate swelling by the macro-porosity and the transition from crystalline to osmotic swelling processes, a factor, termed here the internal strain factor (Υ (-)), is included in the calculation of the hydraulic stress:

$$\sigma_H = \Upsilon(Ss_{fs}) \quad (4.86)$$

where s_{fs} is the total free swell suction (Pa), and S is the saturation (-).

Assuming that the Bishop's parameter χ is equal to saturation this can be substituted into Equation 4.85 to give the effective stress description of the soil as:

$$\sigma' = (\sigma - u_a) + \Upsilon(\chi s_{fs}) \quad (4.87)$$

This is comparable to the Biot constant application (α_B) in the modified effective stress parameter σ'' used to model deformable porous media [Lewis and Schrefler, 1998]:

$$\sigma'' = (\sigma - u_a) + \alpha_B(\chi s_{fs}) \quad (4.88)$$

In unsaturated non-expansive soils Biot's constant is a proportionality factor between the suction pressure of the fluid in the pore caused by the capillarity effect, and the effective stress that is responsible for volumetric deformation. This factor is used to account for deformable porous media when the pore fluid pressure exerts a stress on the soil skeleton. However, Agus et al. [2010] indicate that the dry density of bentonite, and therefore pore space size and shape, has a minimal contribution to the total suction. They conclude that suction pressure in an expansive soil is dominated by the physico-chemical hydration forces within a clay aggregate. Following the interpretation that the hydrating fluid is taken up into the clay aggregates in preference to filling the macro-porosity [Kröhn, 2003], the influence of fluid pressure in the macro-pore is minimal. It therefore follows that the suction pressure in unsaturated bentonite does not have the same affect on the clay aggregate as might be expected by the application of the Biot constant because the suction of a grain can be considered to be in equilibrium with the stress conditions and its volume i.e. suction is not applying a force to the grain in addition to that of the physico-chemical force internally present. Instead, the influence of the intra-aggregate suction pressure is dominant and the swelling processes of aggregates defines the translation of suction change to total effective stress. Consequently the Biot constant is deactivated and the internal strain factor, varied as a function of the water content, is used as a replacement.

Instead of representing an effect of pore fluid pressure, the internal strain factor therefore represents the coupled hydro-mechanical effect of the double structure of porosity observed in bentonites and the swelling mechanism operating at different water contents [Agus, 2005, Lloret et al., 2003, Madsen and Müller-Vonmoos, 1989, Navarro et al., 2015, Pusch and Yong, 2006, Wayllace, 2008]. Furthermore, this process is dry density dependent because the volume of macro-void space that can accommodate expanding clay clusters is reduced for a highly compacted sample in comparison to a low dry density sample (Figure 4.7) [Agus, 2005, Agus et al., 2010, Lloret et al., 2003, Saba et al., 2014, Wang, 2012, Wang et al., 2012, 2014].

4.6.2 Staggered HM Scheme

The HM coupling is implemented through a staggered HM scheme whereby the hydraulic process is solved separately from the mechanical process. This dependency of the hydraulic solution on the mechanical solution, and vice versa, creates significant non-linearity in the calculation of the coupled process as the mechanically calculated confining stress influences the amount of water that can be uptaken, and the amount of water that can be uptaken influences the build up of stress:

$$s = f(\sigma_c) \quad \sigma_c = f(\Delta s) \quad (4.89)$$

In order to overcome this non-linearity in the coupling, a Picard iteration loop between

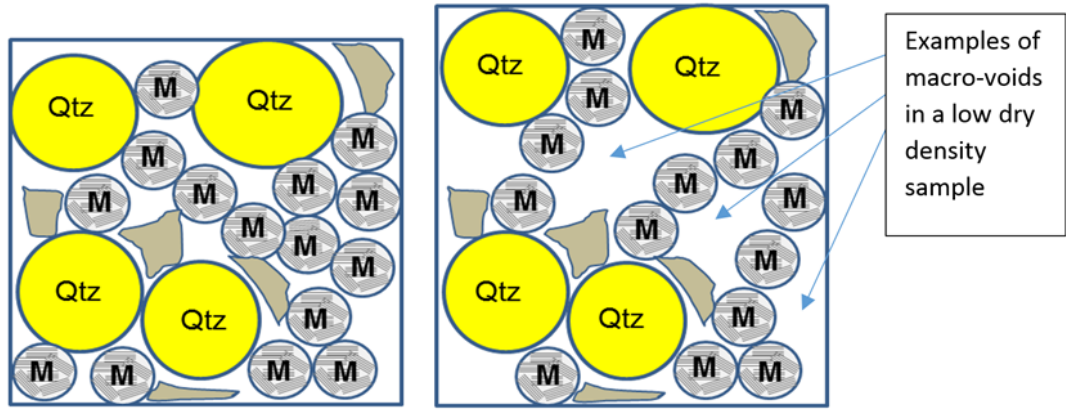


Figure 4.7: Schematic representations of the macro-scale pore space in bentonite-sand mixtures of different densities, modified after Agus et al. [2010]. A high dry density sample (left) has fewer macro-voids than a lower dry density sample (right) and as such transfers more suction change to mechanical stress in the high suction range. M refers to montmorillonite clusters, Qtz refers to quartz particles, and the finer material is silt sized particles.

the two processes is implemented that uses the net mean stress (p), as the dependent variable. The difference in confining stress between two iterations of Richards flow and the mechanical process provides the error criterion that can be tested against a user defined tolerance:

$$|err| = \sigma_c^i - \sigma_c^{i-1} \quad (4.90)$$

$$convergence = \begin{cases} \text{true} & \text{for } |err| \leq \text{tolerance} \\ \text{false} & \text{for } |err| > \text{tolerance} \end{cases} \quad (4.91)$$

The staggered HM scheme is shown in a flow chart in Figure 4.8. Richards' process is solved first to determine the change in suction pressure that contributes to the mechanical process. This is then included in the solve of the mechanical solution, along with any external forces, to calculate displacements and subsequent stress distribution. The stress distribution provides the confining stress acting on the sample for the given change in suction and external stress. However, as the processes do not physically happen one after the other the effect of increased stress with reducing suction must be considered. Consequently the solution is run again with the new confining stress applied to the hydraulic solution. This calculates a different change in suction for the same boundary conditions and time-step, and consequently a different displacement and stress distribution in the mechanics. This iteration loop is repeated until the change in the confining stress is within a pre-defined tolerance limit.

Once convergence is achieved the calculated suction from the hydraulics is a function of the mechanical stress, which is influenced by the change in suction. From the final solution, the mesh is updated and the strain dependent parameters of porosity (n), void ratio (η), dry density (ρ_d), and, in the next time-step, the elastic modulus (E) are recalculated.

Free swell suction is not calculated by Richards' calculation if a pressure based form of the equation is used with the concept of Dueck suction, and therefore is determined from rearranging equation 4.79.

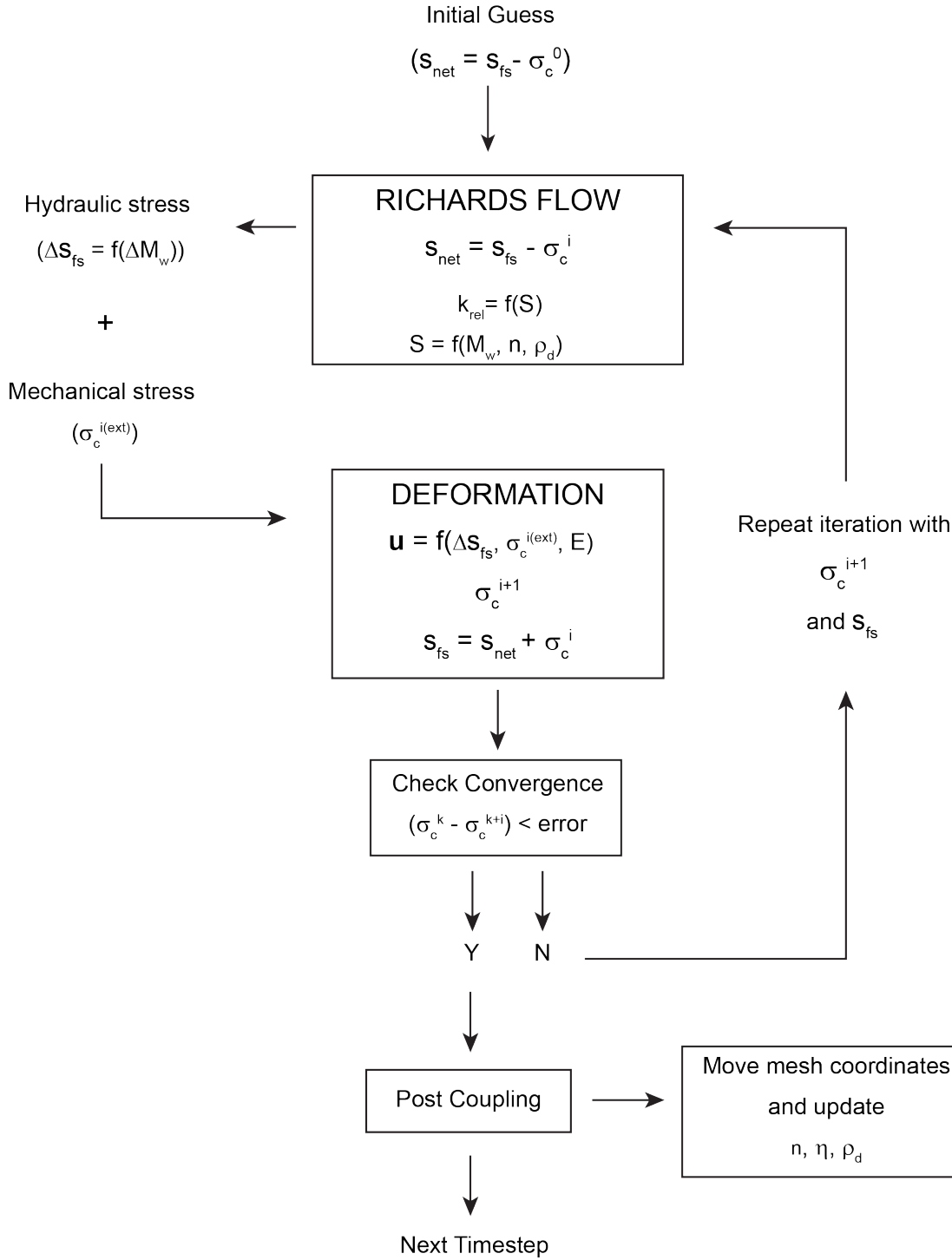


Figure 4.8: A flow diagram illustrating the staggered coupling procedure for Richards' Flow and non-linear elastic processes implemented. The suction pressure is a function of the confining stress and the calculated stress is a function of the change in suction. Consequently an iterative procedure is required to determine the suction pressure, displacements, and mechanical stress for the current time-step. In this diagram s_{fs} is the free swell suction pressure (Pa), s_{net} is the net suction pressure (Pa), M_w is the water content (-), k_{rel} is the relative permeability (m^2), σ_c is the confining stress (Pa), $\sigma_c^{i(ext)}$ is the confining external stress (Pa) e.g. a load, u is the calculated displacement vector (m), n is the porosity (-), ρ_d is the dry density (kg/m^3), η is the void ratio (-), and E represents the material mechanical properties. The superscripts i and $i-1$ refer to the iteration number

4.7 Moving Finite Element Mesh

The finite element method calculates the solution to the unknown field variable by discretising the governing equations over a mesh consisting of nodes and elements. In hydraulic and mechanical processes commonly the solution to the governing equations provides the user with an understanding of some motion e.g. the flow of water or the deformation of a solid, or in this case the flow of water in a deforming solid. The finite element approach to problems such as this falls into the study area of continuum mechanics. This section introduces the concept of moving finite element mesh techniques, the method implemented in this model, and the specific considerations required for the application to the varying hydro-mechanical conditions in the SEALEX experiments.

Numerical procedures within this field commonly fall into one of three categories; Lagrangian, Eulerian, or arbitrary Lagrangian-Eulerian [Donea et al., 1999]. In Lagrangian procedures the mesh nodes move with the calculated motion of the material particle, whereas the Eulerian procedures maintain a constant location of the node but calculate the motion of the material particle with respect to the stationary (fixed) mesh. The arbitrary Lagrangian-Eulerian (ALE) method aims to combine the two end members by allowing the mesh nodes to move but without the restriction that they must follow the exact motion of the particles [Donea et al., 1999]. The ALE method can be used as either end member method but also as a combination where the mesh can move but does not necessarily follow the motion of the particles. In order to move the mesh in a motion that does not directly follow the particle motion a form of mesh-displacement algorithm is required to define the mesh-node velocities or displacements at each update step. These algorithms generally fall into two main categories; mesh regularisation or mesh adaptation [Donea et al., 1999].

4.7.0.1 Mesh Regularisation

Mesh regularisation is essentially a geometric control on the shape and size of the elements in the mesh so that mesh distortion problems do not arise. A number of methods have been proposed including the transfinite mapping method, Laplacian smoothing and variational methods, and mesh smoothing by averaging or interpolation [Donea et al., 1999]. Stein et al. [2003] present a method of a moving mesh for deformations of fluid-structure interactions based on elastic deformation and a control function based on the change in area and shape of the element. Liao and Xue [2006] propose the deformation method that prescribes a fixed value for the determinant of the Jacobian i.e. the element area, and therefore ensure the element area is non-zero and positive.

4.7.0.2 Mesh Adaptation

Adaptive techniques fall into three main categories based on their adaptive methods:

- the h -method refines or coarsens the mesh based on *a priori* error indicators and involves re-meshing or updating element connectivity with each time-step,
- the p -method selects the polynomial degree used in the FE approximation based on the smoothness of the solution and focusses the higher order polynomial degree in the area of most change, and

- the r -method moves the nodes towards the area where refinement is required and ensuring element connectivity without re-meshing [Zegeling, 1998].

Each of these methods aims to increase the mesh density in the regions in which the finite element solution changes most rapidly and reduce density in regions where little change occurs, and they are commonly based on some form of estimate of solution accuracy or complexity [Stein et al., 2003, Zegeling, 1998].

Mesh regularisation and adaptivity both ensure the mesh cannot become entangled or cause element inversion [Donea et al., 1999]. Element inversion occurs when a node from one side of the element ‘overtakes’ the opposite side of the element e.g. for an equilateral triangle if the bottom-left node becomes the top-right node then the triangle has a reversed orientation [Liao and Xue, 2006]. This is a potentially significant problem for description of motion via the Lagrangian method.

In the developed HM model the movement of the mesh is linked to the mechanical properties of the material through the strain dependent non-linear elastic function. Due to the explicit calculation method employed, the coupling of the mesh movement to mechanical properties could lead to potential mesh instability caused by entanglement or inversion at low mechanical stiffness. In order to overcome this potential drawback of the Lagrangian method, the minimum elastic modulus threshold function is introduced, as described in Section 4.5.1. In addition, the time-step length is manually controlled in order to reduce the possibility of large strains occurring in a single time-step. These measures allow the Lagrangian method to achieve good mesh stability.

4.7.1 Moving Mesh development

The main motive for implementing a moving mesh is to track the deformation of the sample and provide a method to record deformation dependent elemental properties. A Lagrangian moving mesh is chosen and implemented to describe the motion of the solid i.e. the mechanical deformation. This enables the update of material properties for use in the non-linear elastic mechanical model and provides a method for simulating large deformations with a model based on the infinitesimal small strain theory. One of the key advantages of the Lagrangian method is that it allows the simulation of materials with history dependent constitutive relationships [Donea et al., 1999], which are common in the soil mechanics field [Alonso et al., 1990, Nguyen et al., 2005, Rutqvist et al., 2005].

In soil mechanics applications moving meshes are not commonly used because non-recoverable strains are often accounted for by plasticity, and elastic deformations are reversible and independent of strain history. This means that the mesh can be kept constant and calculations performed for the total stress up to that time-step. However, a moving mesh lends itself well to a non-linear elastic approach where the strain history of the sample can be directly incorporated and non-recoverable strains calculated [Donea et al., 1999].

The moving mesh implemented here is based on updating the mesh node locations as a function of the calculated mechanical displacement using the following procedure:

- At the end of each mechanical calculation the calculated displacements are added to the nodal coordinates (Figure 4.9).

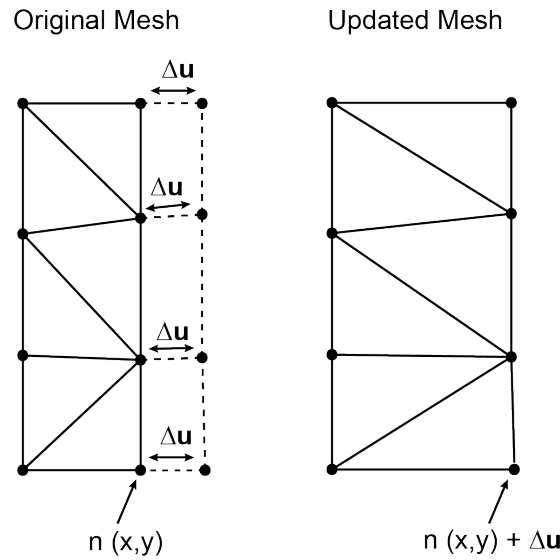


Figure 4.9: Schematic diagrams showing the addition of the calculated displacements to the nodal coordinates to produce a new mesh each time-step.

- The subsequent coordinates are then set to the mesh nodes to produce an updated mesh for the next time-step.
- Each element is then configured from the updated mesh node coordinates.

For the calculation of the finite element scheme the Jacobian coordinate transformation uses the updated mesh node coordinates so the solution sees an essentially new mesh each time-step. This Lagrangian moving mesh method ensures element connectivity is preserved. However, it can be susceptible to element inversion and/or entanglement and requires careful consideration of the time-step length in combination with the mechanical model parameters to ensure mesh stability. The moving mesh application is activated in the input files in the process file using the keyword \$DEFORMING_MESH.

4.7.2 Implications for hydraulic calculations

In contrast to the Lagrangian moving mesh employed for the mechanical solution, the hydraulic solution is approached in an explicit Eulerian method such that the motion of the fluid is calculated with respect to the fixed grid for that time interval. However, the iterative procedure of coupling the hydraulic and mechanic processes in a staggered HM scheme means that each loop of the hydraulic processes corresponds to a different effective stress. This has two impacts on the hydraulic process; firstly the water retention properties may vary between iterations as a function of the confining stress, and secondly the different effective stress could result in different sample volumes. Therefore, as the hydraulic solution is not only dependent on the stress but also volumetric properties such as dry density, porosity, and saturation, the volumetric change associated with the change in effective stress needs to be incorporated into each loop of the hydraulics. To achieve this, a 'virtual' mesh is implemented which is updated for each iteration loop of the hydraulics.

The virtual mesh is separate from the global mesh and only applies to the hydraulic process. It is built with the following procedure at the end of each mechanical process loop:

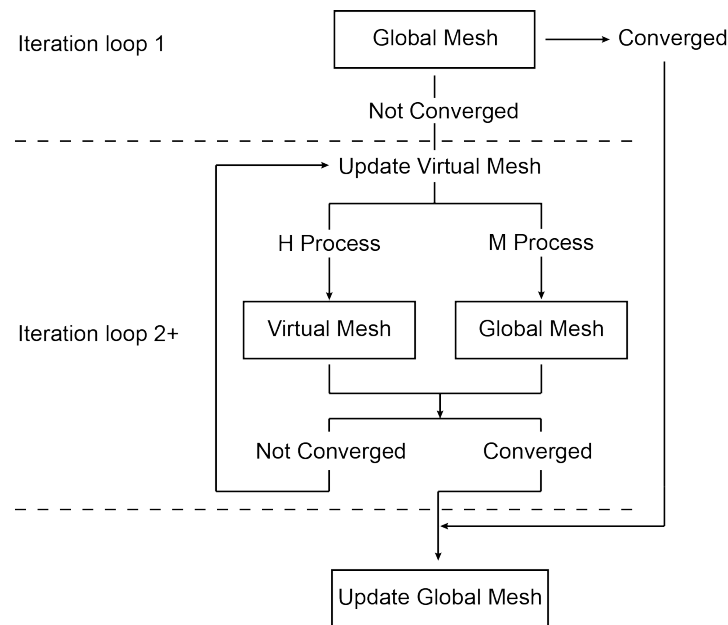


Figure 4.10: A flow diagram illustrating the use of the virtual mesh. The time-step starts with the global mesh and calculates a solution to the hydraulic and mechanical processes. If the solution does not converge the calculated displacements are used to update the virtual mesh. The hydraulic solution for the next iteration loop is calculated over the virtual mesh (corresponding to the effective stress conditions from the previous loop mechanical solution), but the mechanical solution is calculated over the start-time-step global mesh. Once convergence is achieved the global mesh is updated with the calculated displacements.

- Calculated displacements are added to nodal coordinates.
- These coordinates are set to virtual mesh nodes to produce the virtual mesh for the hydraulic solution.
- Each virtual element is configured from the virtual mesh nodal coordinates.
- Element properties of porosity, dry density, and void ratio are updated as a function of the new virtual element volume.

The result of the iterative procedure is that, at convergence, the virtual and global meshes coincide and the next time-step begins with a single mesh (Figure 4.10). The inclusion of the virtual mesh is shown in the iterative coupling procedure in Figure 4.11 and is activated in the process input file using the keyword `VIRTUAL` underneath `$DEFORMING_MESH`.

4.7.2.1 Geometry considerations

The current release of OpenGeoSys (version 5) is programmed for a constant/fixed mesh application and as such the geometric objects defined by the user in the .gli file are fixed for the duration of the solution. Therefore, for this moving mesh technique this leads to problems when trying to access data from specific points or polylines. As this project is concerned with both constant volume and volumetric expansion these problems fall into two main categories; when the mesh moves over a data output point that is required to be constant, and when the data output is required to move with the moving mesh. These problems are restricted to the

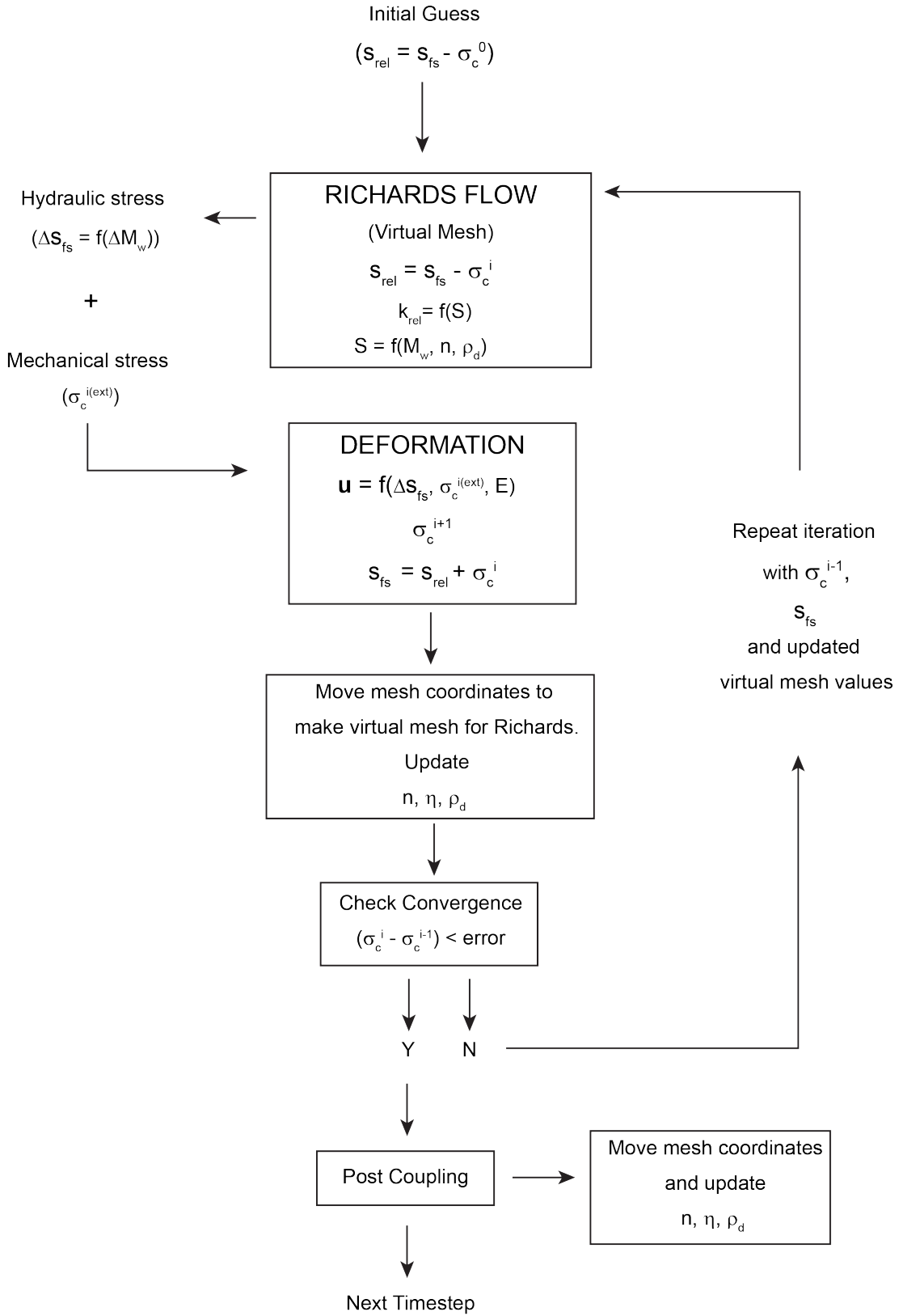


Figure 4.11: A flow diagram illustrating the iterative procedure used to calculate the coupling between the hydraulic and mechanical processes. The virtual mesh used to update the volume dependent hydraulic parameters is calculated after the deformation process and before convergence is checked. All symbols are the same as in Figure 4.8.

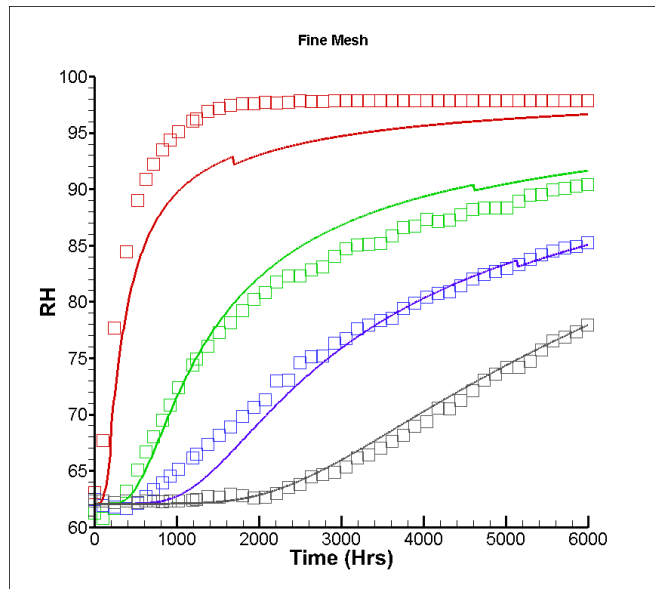


Figure 4.12: Infiltration test results from a moving mesh model with fine grid size. Without the interpolated point output the movement of the mesh over the geometric point results in a jump in the output data.

output of data because within the process iterations geometric entities, such as a polyline, use the mesh nodes as opposed to the geometric nodes. Therefore, because the polyline remains comprised of the same mesh nodes throughout the solution the updated coordinates of the mesh nodes are used (both virtual and real depending on the process).

4.7.2.1.1 Interpolated Point

The first geometric consideration is when an output point is defined as constant but the mesh moves during the simulation. The fixed mesh implementation of data output at a geometric point searches for the nearest node to the point and copies that nodal value of the variable into the output file. In fixed mesh applications this is not a problem because the node closest to the geometric point remains constant throughout the simulation. However, if the mesh moves during the simulation then the nearest node to the geometric point may change leading to a jump in data if there is a gradient in the variable across the element. This is seen if the fixed point geometric objects are used in the simulation of the infiltration test (as described in Chapter 5) shown in Figure 4.12.

In order to overcome this problem the data supplied to the geometric point must be interpolated from the nodes of the element in which it is present. For triangular elements this is relatively straight forward but is more complicated for rectangular elements. As the moving mesh implementation is based purely on the calculated nodal displacements it makes no discrimination on element type. The base 2D elements to the commonly used 3D elements of tetrahedra and hexahedra are the triangle and quadrilateral. For the sake of flexibility and for future development of the technique if 3D simulations are required, both triangular and quadrilateral elements are considered and implemented. However, as modelling was performed with triangles in the main, the implementation of the interpolated point value in triangle elements is presented here. The correct interpolation of the data to the geometric points

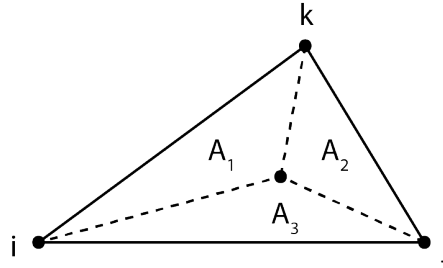


Figure 4.13: A schematic diagram showing the method for the calculation of the area of a quadrilateral element. The sum of areas A_1 , A_2 , and A_3 make up the total area of the triangle element.

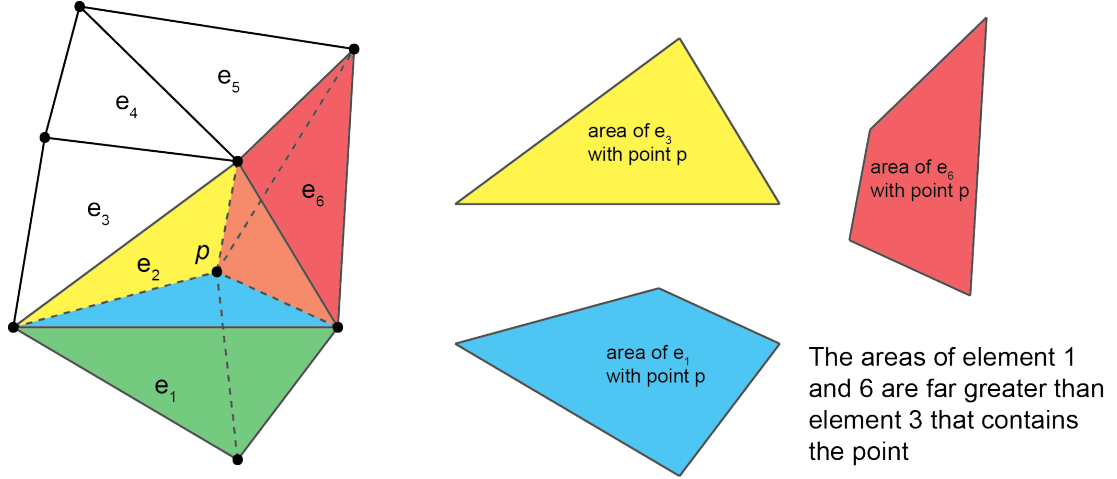


Figure 4.14: A schematic diagram illustrating the difference in areas calculated using the sum of the areas of the triangles made up of each edge of the element and the point location. By comparing the area of every element calculated with the point to the actual element area it is possible to find the element containing the point.

requires two steps if triangle elements are used, and three if quadrilateral elements are used:

- Finding the element the point is located within,
- (If using quadrilateral elements) Applying an inverse coordinate transformation from the global coordinates of the geometry point (which stays constant throughout the simulation) into the local coordinates, and
- Interpolating the value of the field variable to the point.

Finding the element the point is located in can be achieved by finding the sum of the internal areas of the triangles made by the point location and each edge of the element for each element. The area of each element is also calculated separately, either as half the determinant of the Jacobian matrix or as a sum of the triangles made by the element centre and each edge of the element, as shown in Figure 4.13. For all but the correct element the point will be located outside the bounds of the element and therefore the sum of the areas will be larger than the actual area of the element. By comparing the area of each element calculated from the sum of the areas including the point to the actual element area, the correct element can be found. This is illustrated by Figure 4.14.

Once the correct element has been found, an analytical solution exists for the interpolation of the nodal values to any point within a triangular element so the inverse coordinate transformation from global to local coordinates that is required for quadrilateral elements [Hua, 1990] is not necessary [Istok, 1989].

4.7.2.1.2 Triangular element interpolation

The analytical interpolation method is well explained in Istok [1989]. The global coordinates of the point and the element nodes are known so all that is required is to interpolate the known node values to the point within the element. The interpolation functions from each node to the point p in Figure 4.15 are defined as [Istok, 1989]:

$$\begin{aligned} N_i^{(e)}(x_p, y_p) &= \frac{1}{2A}(a_i + b_i x_p + c_i y_p) \\ N_j^{(e)}(x_p, y_p) &= \frac{1}{2A}(a_j + b_j x_p + c_j y_p) \\ N_k^{(e)}(x_p, y_p) &= \frac{1}{2A}(a_k + b_k x_p + c_k y_p) \end{aligned} \quad (4.92)$$

where A is the element area, x_p and y_p refer to the cartesian coordinates of the point p , and i, j , and k refer to the nodes shown in Figure 4.15. The interpolation functions at the point are constrained by the rule that:

$$N_i^{(e)}(x, y_p) + N_j^{(e)}(x_p, y_p) + N_k^{(e)}(x_p, y_p) = 1 \quad (4.93)$$

The values of a , b , and c for each node are calculated as:

$$\begin{aligned} a_i &= x_j y_k - x_k - y_j & a_j &= x_k y_i - x_i y_k & a_k &= x_i y_j - x_j y_i \\ b_i &= y_j - y_k & b_j &= y_k - y_i & b_k &= y_i - y_j \\ c_i &= x_k - x_j & c_j &= x_i - x_k & c_k &= x_j - x_i \end{aligned} \quad (4.94)$$

The value of the primary variable e.g. suction (s), calculated at each node is then interpolated across the element to point p by:

$$s_p = N_i^{(e)} s_i + N_j^{(e)} s_j + N_k^{(e)} s_k \quad (4.95)$$

This can be expressed for an element of n nodes as:

$$s_p = \sum_{i=1}^{i=n} N_i s_i \quad (4.96)$$

If data is required at an interpolated point this is activated by naming the point 'INTERPOLATED.POINT.point_name' and including the same name in the output files.

4.7.2.1.3 Moving Point

The second consideration for data output is when the required information is from a location in the sample that moves e.g. calculating the displacement at the top surface of a sample as it expands. For this output requirement the constant geometric point is not suitable and an

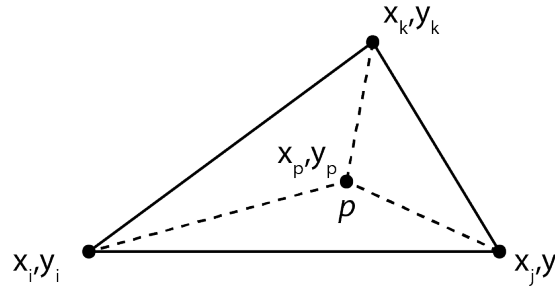


Figure 4.15: A diagram of a linear triangle element containing the point p . Nodal values of the output variables are interpolated across the element to point p using the interpolation functions in Equation 4.92.

alternative method is needed. In order to allow the data from a specific point that moves with the mesh the geometric point must be mapped to the closest mesh node.

If a moving point is required then this needs to be specified in the user input. The point must be named 'MOVING_POINT_point_name' as this is the switch used in the output function. Activating a moving point output results in the geometric node being mapped to the mesh node during the initialisation of the model. This then remains assigned to the same mesh node throughout the simulation and can therefore move with the mesh.

4.7.2.1.4 Polyline

A polyline is a geometric object defined in the .gli file that joins a series of points together. In the same way that the geometric points are defined during the model initialisation for a fixed mesh, the points on the polyline and the distances between them are constant for the duration of the solution. The mesh node IDs are also defined at the initialisation stage so the polyline is always composed of the same nodes. However, in certain applications it may be important to know the actual distances between the points on a polyline for integration purposes and post simulation calculation of variables, such as flux. Therefore it is considered important to be able to output the updated mesh coordinates of the polyline nodes.

Polylines are commonly used to apply boundary conditions or source terms as well as output data. In the process iterations the boundary conditions and source terms are applied to the mesh nodes (not the geometric polyline points) because the functions find the mesh nodes on the polyline. This results in the application of the boundary condition or the source term to the updated mesh coordinates.

For output of the updated polyline distance an extra function to calculate the distance between the mesh nodes is included. This function is activated by the \$DEFORMING.MESH keyword in the process file.

4.8 Summary of implementation in OpenGeoSys

The mathematical model described in this chapter has been implemented in OpenGeoSys and has involved a significant amount of code development to extend OGS for this application. In this section, these developments are summarised in the context of the object orientated structure of the code shown in Figure 4.1, repeated here for convenience (Figure 4.16). A more

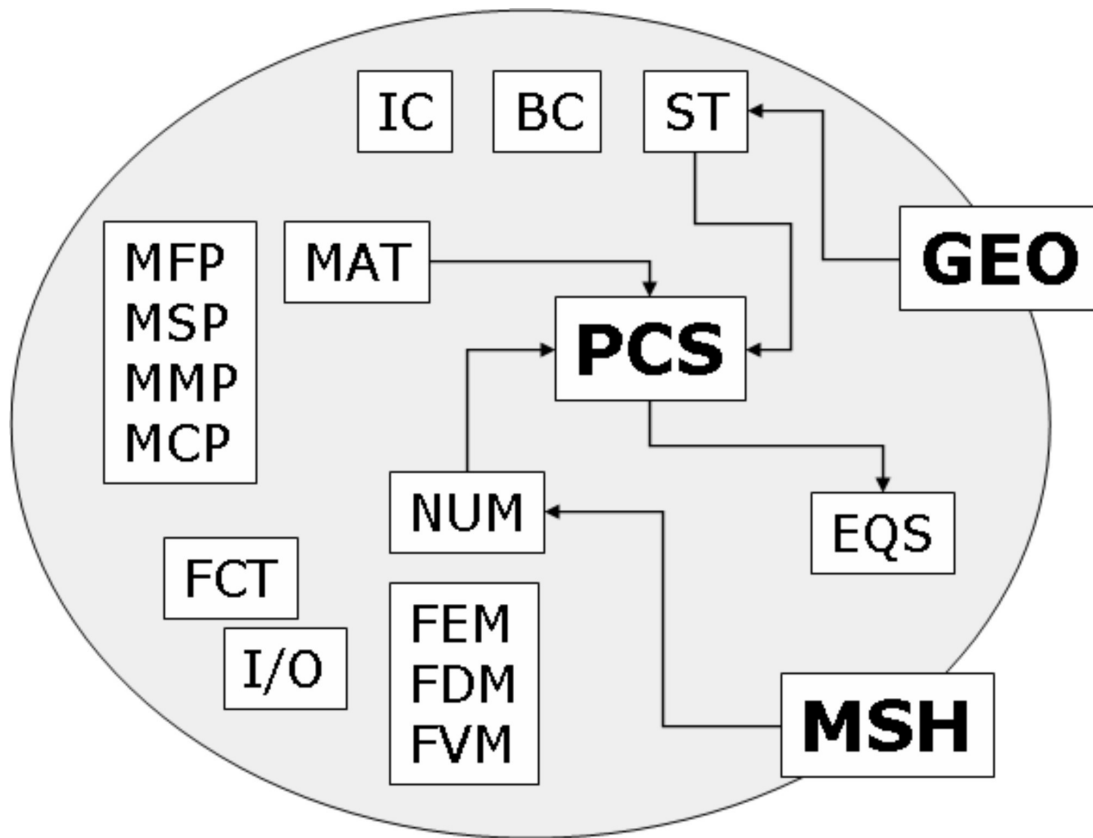


Figure 4.16: The file structure and necessary inputs required to run a model in the object oriented code OpenGeoSys [Kolditz et al., 2012]

detailed description of the developments can be found in Appendix A along with the digital appendix of the source code.

The main developments with reference to Figure 4.16 are:

- **GEO:** Capability has been extended to include new geometric point names to allow the INTERPOLATED_POINT and MOVING_POINT to be included in the output.
- **MSH:** The mesh developments have been discussed previously in this Chapter but a summary list is included here:
 - Updating mesh coordinates to create a Lagrangian moving mesh with respect to the mechanical solution.
 - Creating a separate virtual mesh that deforms within time-step iterations. This is developed to provide consistency in hydraulic calculations that depend on element volume properties e.g. porosity and permeability.
 - Definition of element property variables that vary as a function of strain i.e. porosity, dry density, void ratio, and Young's Modulus.
 - Specific functions to update these strain dependent element variables both for the virtual mesh (intra-time-step updates) and the master mesh (inter-time-step updates).

- Set up of new member functions to extrapolate the non-linear strain calculations from the Gauss points to the nodes in order to maintain current functionality within the code and extend functionality to a Lagrangian moving mesh.
- **NUM:** The numerical solution procedure has been developed to include the coupling of the hydraulic and mechanical process. The iterative coupling procedure has been developed to be based on the net mean stress because of the strong coupling between the stress developed as a result of hydration in confined conditions, and the amount of hydration change that can occur due to the stress conditions.
- **BC:** Displacement dependent boundary conditions employing the moving finite element mesh have been implemented for both 2D axisymmetric and 2D plane strain cross-section models. These include the determination of the number of active nodes along the polyline to which the boundary conditions are applied.
- **MSP:** The strain dependent non-linear elastic function has been implemented in the material solid properties class as a new member function specific to this model. In addition, the internal strain factor determining the contribution of a change in suction to the calculated stress is developed and implemented.
- **MMP:** The material medium property class functionality has been developed to include a number of specific functions for both a moving mesh and bentonite modelling. These include:
 - The implementation of Dueck suction in the saturation - suction pressure relationship.
 - The conversion of the derivative of pressure with respect to saturation into the derivative of pressure with respect to water content, as discussed in this Chapter. This allows the experimentally derived free swell curve to be used directly as input, and to incorporate volumetric dependency into the water retention behaviour.
 - Implementation of a variety of permeability models to investigate the porosity and dry density dependence of the saturated intrinsic permeability.
- **I/O:** The output capability has been extended to aid visualisation of the model results. This includes:
 - Extrapolation of the strain dependent parameters such as porosity, void ratio, elastic modulus, water content, saturation, swelling pressure, and dry density.
 - Specific geometric considerations (as described in Section 4.7) including the INTERPOLATED.POINT and MOVING.POINT, and polyline length.

Chapter 5

Modelling Step 1 of the SEALEX experiments

In this Chapter the coupled hydro-mechanical model described in Chapter 4 is calibrated against a series of laboratory tests conducted by the Institut de Radioprotection et de Sûreté Nucléaire (IRSN) [Wang, 2012]. The Dueck suction concept is first shown to be suitable to describe the stress-dependent water retention properties of the free swell and constant volume water retention tests, before the hydraulic model is calibrated to a constant volume infiltration test. A number of permeability models are tested and it is found that the Liu et al. [2011] model produced the best results. Its applicability for use with bentonite modelling is also demonstrated by the simulation of a bentonite of different composition (GMZ bentonite [Ye et al., 2009]). The non-linear elastic model is calibrated to controlled suction consolidation tests and is able to reproduce the non-recoverable strains exhibited in experiment.

5.1 Introduction

The SEALEX experiments comprise both small scale laboratory tests and full-scale *in situ* experiments on compacted bentonite-sand blocks that make up a prototype hydraulic seal. The aims of the SEALEX experimental program are to investigate the long-term hydraulic performance and changes in external confining conditions e.g. concrete plug failure [Barnichon et al., 2012]. The experiments increase in complexity from the standard soil mechanics laboratory tests to the full scale *in situ* experiments and provide a good framework for the development and testing of numerical models. As such, they have been chosen to form the experimental data for Task A of DECOVALEX-2015 with the following steps specific to the bentonite behaviour:

- Step 1 - Soil mechanics laboratory tests of consolidation, infiltration, and water retention
- Step 2 - $1/10^{th}$ scale mock-up test of the *in situ* experiments
- Step 3 - Full scale *in situ* experiment

This work is focussed on the parameterisation of the non-linear elastic bentonite model described in Chapter 4 and its application to the modelling of steps 1, 2, and 3. Figure 5.1

shows the different experiments undertaken and their respective challenges for the numerical modelling of each scenario.

The laboratory tests of the SEALEX experiments provide the data for model calibration in Step 1 of the DECOVALEX 2015 Task A project. A number of controlled variable tests were conducted to aid parameterisation and/or development of models for both hydraulic and mechanic processes. These include an infiltration test, a water retention test, and a number of consolidation tests on samples held at different imposed suctions. The modelling approach was to first tackle each test as a single uncoupled process problem before hydro-mechanical modelling was considered [Bond et al., 2014]. The controlled nature of the laboratory cases allows the separation of the strong HM coupling in order to parameterise the individual processes. However, due to the strong inter-dependence of the hydraulic and mechanical processes, HM coupling was necessary in order to model more complex scenarios e.g. subsequent steps in the DECOVALEX Task. This chapter discusses the application and calibration of the coupled HM model developed in Chapter 4 to the laboratory experiments from Step 1 of DECOVALEX-2015 Task A.

5.2 Water Retention Curve

The hydraulic process is approximated using Richards' equation for unsaturated fluid flow driven by a suction pressure gradient, as discussed in Chapter 4, and therefore requires the description of the suction-saturation relationship to complete the equation (Equation 4.7). This is commonly termed the water retention curve and is determined experimentally. The water retention curve has been shown to be a sensitive parameter in the modelling of unsaturated soils [Fredlund et al., 2012, Fredlund, 2002]. Typically the relationship is derived in terms of suction and gravimetric water content and then converted to a saturation for use within constitutive equations of flow. Commonly, for non-expansive soils, the constant volume water retention data are then fitted with characteristic water retention functions such as the van Genuchten relationship [van Genuchten, 1980] or Brooks and Corey function [Brooks and Corey, 1964]. However, in expansive soils the degree of saturation may vary depending on the sample volume, so the SEALEX experiments provide both constant volume and free swell condition water retention curves for calibration of suction-water content relationships. A pre-compacted bentonite sample with a dry density of 1.67 Mg/m^3 and initial gravimetric water content of 11% was placed into a cell and hydrated to a range of imposed suctions. The experiments investigated suctions ranging from 309 MPa to 0.01 MPa for free swell conditions and 65 MPa to 0.01 MPa for constant volume conditions [Wang, 2012]. Consequently, the vapour equilibrium technique was used to control suction in the range of 309MPa - 4.2MPa, and an osmotic method was used at suctions $<4.2 \text{ MPa}$. The water retention curve is then constructed from the gravimetric water content measured at each suction once the sample is at equilibrium and the experimental results are shown in Figure 5.2 [Wang, 2012].

5.2.1 Conceptual Interpretation of Experimental Results

The free swell water retention data in Figure 5.2 exhibit a typically bi-modal behaviour common to many expansive bentonite materials [Marcial et al., 2002]. Interpretation of this behaviour with regards to the swelling process suggests that at high suction the water uptake

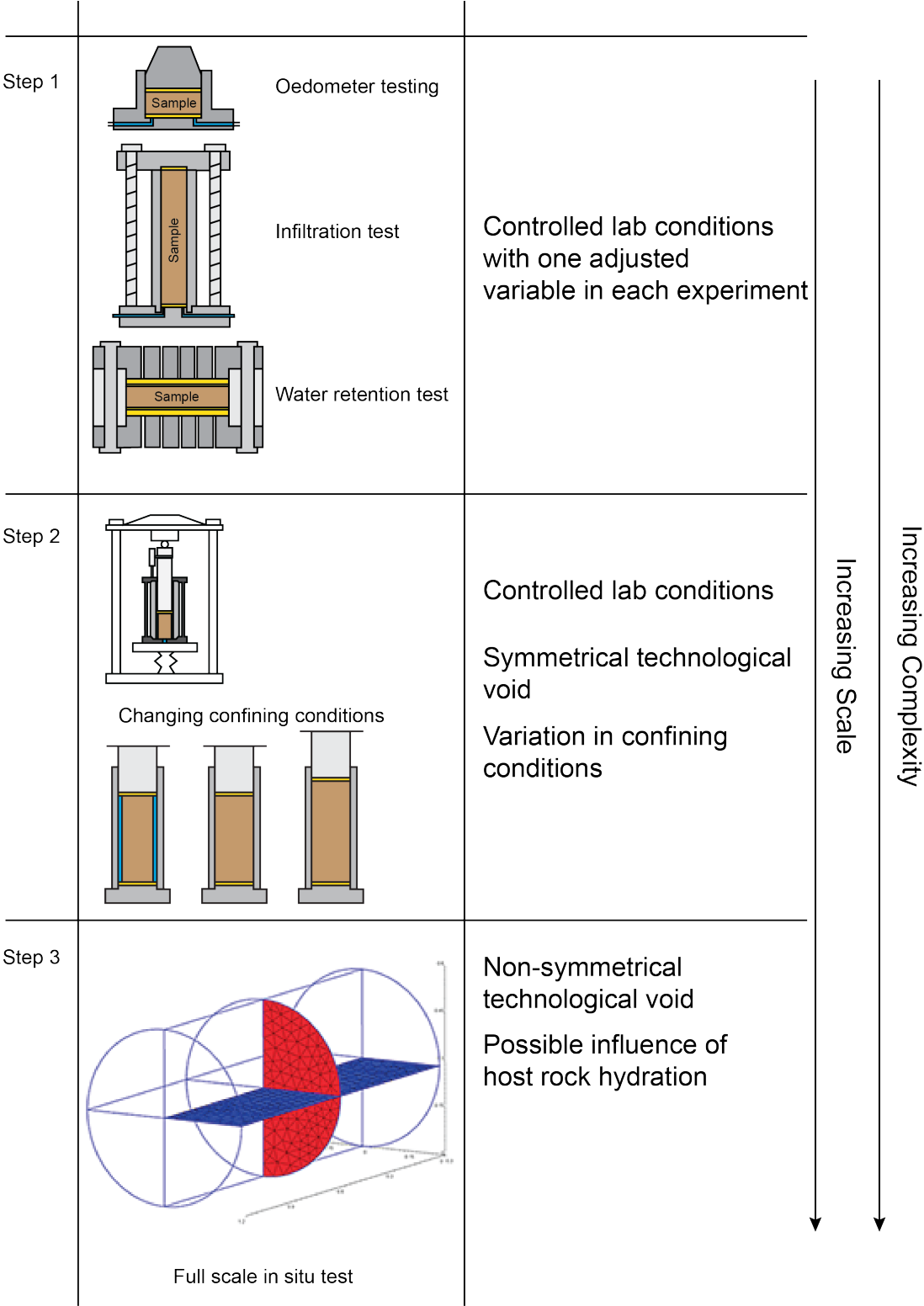


Figure 5.1: A representation of the increasing complexity and scale of the experiments undertaken as part of the SEALEX programme and their modelling challenges.

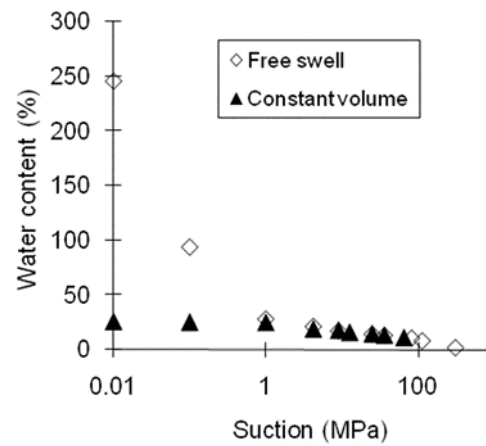


Figure 5.2: Experimental results for the water retention curve under free swell and constant volume conditions in the SEALEX laboratory tests [Wang, 2012]

is dominated by hydration forces associated with crystalline swelling [Likos and Lu, 2006, Wayllace, 2008]. As suction reduces and swelling proceeds, this process gives way to osmotic suction that leads to a greater volume change and water uptake [Wayllace, 2008]. Consequently, the volume expansion and continued water uptake mean that a sample in free swell conditions has a constantly evolving saturation. In comparison, under constant volume conditions the water uptake is limited by the volume of the void space within the sample and the hydration cell (Figure 5.2). In this instance, saturation can be reached and the data calibrated to with a standard function, such as the van Genuchten function. However, in the SEALEX experiments volume change is expected, and as such, the variation of water retention properties with volume must be accounted for.

Considering both the free swell and constant volume conditions together, it can be observed that the water retention data in Figure 5.2 clearly show a dependency on the stress conditions of the sample. Hydration under constant volume conditions results in the development of a swelling pressure. This has been linked to the difference in constant volume and free swell water retention behaviour by Dueck [2004], as discussed in Chapter 3.

The experimental results also indicate that the volume of water that enters the sample under constant volume conditions is greater than that expected by a mass balance calculation using the initial porosity value. Initial porosity is estimated to be 39.4% from a bentonite dry density of 1.67 Mg/m^3 . Calculating the total mass of water that can fill the voids in the sample volume results in a gravimetric water content of 23.6%. Experimental results indicate that the final gravimetric water content is 24.6%. In order to match the experimental data, either the sample height needs to increase by approximately 0.45 mm, or the density of the water must increase to approximately 1.045 Mg/m^3 . Alternatively, the initial estimate of porosity may be inaccurate, or the pore structure may evolve with hydration e.g. exfoliation of grains may create more pore space within the sample [Pusch and Yong, 2003, Wang et al., 2014]. An increase in sample height has been measured in some experimental procedures as part of the SEALEX experimental programme [Saba, 2014, Wang, 2012], although these are for higher density bentonites with greater swelling pressures, and smaller deformation than would be required to match the experimental mass balance. Jacinto et al. [2012] hypothesised that the

apparent over saturation of bentonite under constant volume conditions may be as a result of a change in water density close to the clay mineral surfaces. Both may be plausible explanations as to the reason that more water than expected is entering the sample under constant volume conditions. The following section describes the modelling method.

5.2.2 Model Set-up and Results

The concept of Dueck suction (as described in Chapter 3) is employed to describe the water retention properties of the MX-80 bentonite-sand mixture used in the experiments. This concept states that the water retention behaviour under confining conditions can be determined from the free swell water retention data and the confining stress [Dueck, 2004, 2008, Dueck and Börgesson, 2007]. As data points are limited in the low suction range due to the large change in water content over a small suction range, an empirical formula after Bond and Benbow [2009] is used to provide a smooth relationship between suction and water content.

$$s_{fs} = M_b(\exp(a - bM_w) + \exp(c - dM_w)) \quad (5.1)$$

where s_{fs} is the free swell suction, M_b is the mass fraction of bentonite in the mixture, and a , b , c , and d are all fitting constants. The empirical fit to the data is then used as input data to define the free swell curve. Experimental data constrained the initial conditions to be 11% water with an initial suction value of c.64.5 MPa calculated from the relative humidity via Kelvin's Law.

$$s_{fs} = \frac{-R \cdot T}{\omega_w \left(\frac{1}{\rho_w} \right)} \cdot \ln RH \quad (5.2)$$

where R is the gas constant ($8.314 \text{ J mol}^{-1} \text{ K}^{-1}$), T is the absolute temperature (K), ω_w is the molecular mass of water (18.016 kg/kmol), ρ_w is the unit weight of water (kg/m^3), and RH is the relative humidity ranging from 0.0-1.0 (-) [Blatz et al., 2008]. The free swell water retention data were fitted with equation 5.1 using the following values; $a = 7.4$, $b = 24.25$, $c = -0.5$, $d = 1.5$. M_b was experimentally defined as 0.7. Figure 5.3 shows the calibration to the free swell water retention data (in red) that formed the input data for the suction-water content relationship.

A 2D axisymmetric triangular mesh was produced in the mesh generating software Gmsh [Geuzaine and Remacle, 2009], and is shown in Figure 5.4. Hydration was modelled with a pressure boundary condition at the base corresponding to the suction pressure of water, and no flow boundaries to the sides and top. In order to maintain constant volume conditions a zero displacement mechanical boundary was applied to all model boundaries. Initial conditions were prescribed as the experimental data of suction (from the relative humidity), porosity, void ratio, and dry density.

Figure 5.3 also shows the results for a fully coupled HM model calculation of the constant volume conditions (blue), which indicates a good agreement to the experimental data. Final gravimetric water content under constant volume conditions calculated by the model is 23.6% which matches the expected value from the initial mass balance calculations. This also compares closely to the 24.6% value for a net suction of 0.1 MPa and corresponds to an error of 4%. As previously discussed from an analytical view point, this error with respect to the data is as a result of the model not capturing the apparent over saturation of the sample under constant volume conditions. This may be as a result of a slight volume change in the experi-

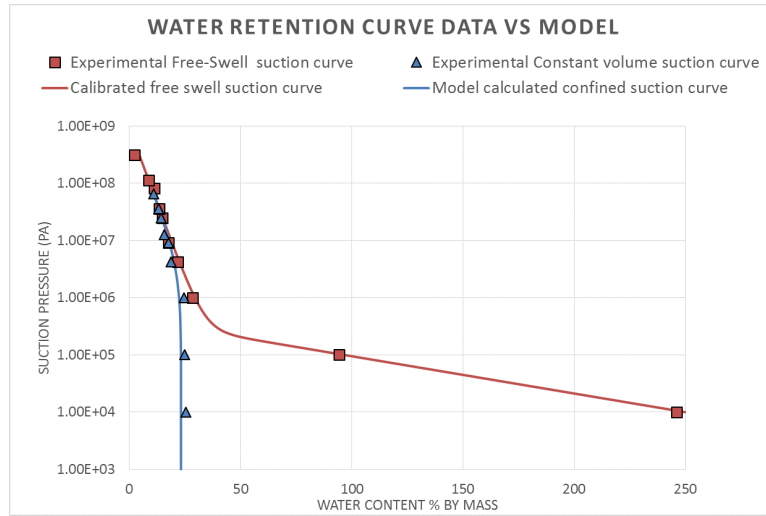


Figure 5.3: The calibrated free swell suction curve (red) matched to the experimental data and the initial conditions. Also shown is the calculated constant volume water retention properties from a numerical simulation (blue) compared to the experimental water retention data for constant volume conditions. This demonstrates the applicability of the Dueck suction method.

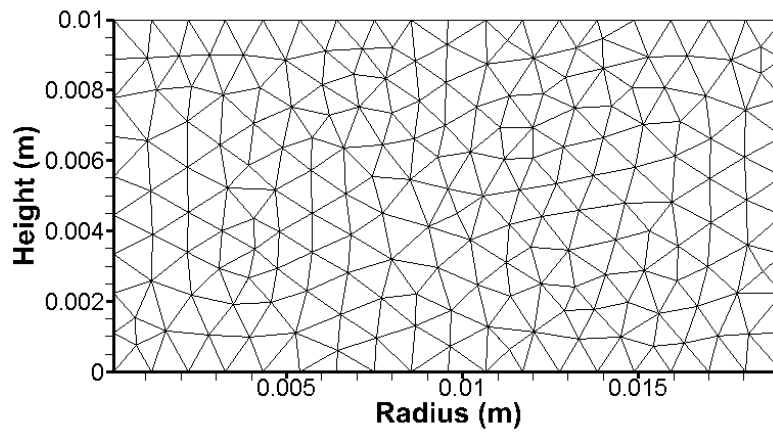


Figure 5.4: The 2-D axisymmetric mesh used for the HM simulation of the constant volume water retention behaviour.

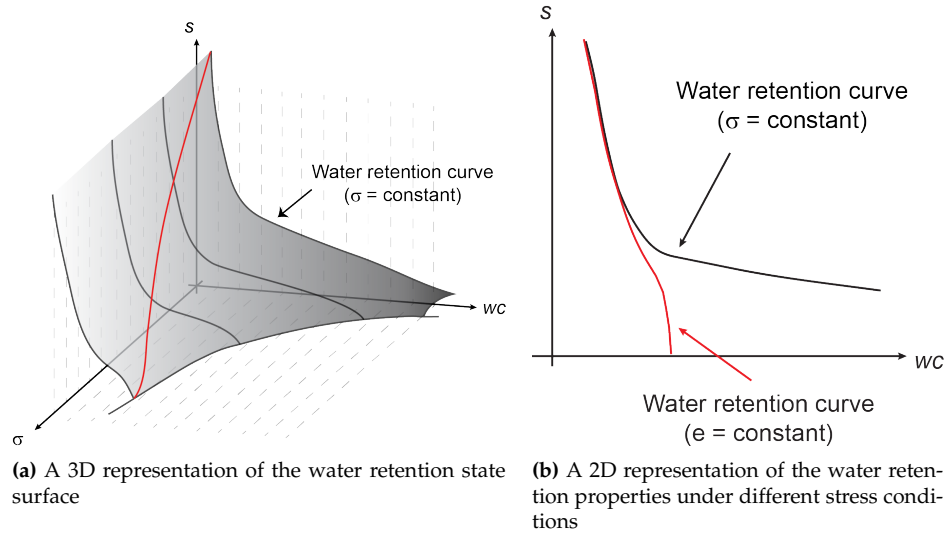


Figure 5.5: Schematic diagrams to represent the effect of the stress conditions under free swell conditions (black) and constant volume conditions (red). The two conditions represent end member behaviours (not including consolidation) and the state surface therefore allows the calculation of the water retention properties for any stress conditions between the two.

mental process not being simulated by the zero displacement boundaries, a variation in water density within the sample not being considered, or not taking into account processes such as exfoliation which may lead to the evolution of porosity as hydration proceeds [Wang, 2012].

These results represent the end member water retention behaviour over the range of stress conditions between constant volume and free swell. This behaviour is fully described by four variables: suction, water content, confining stress, and void ratio. The two main variables are the suction and the water content, while the confining stress and void ratio are coupled variables that reflect the changes to the water retention properties as a function of the stress conditions. For example, if the sample is allowed to swell freely, the suction-water content relationship is viewed in terms of zero confining stress but changing void ratio, whereas if the sample volume is held constant, the suction-water content relationship is viewed in terms of zero volume change but changing confining stress. This is illustrated in Figure 5.5.

The calibration to the free swell curve and calculation of the constant volume water retention just by using the confining stress provide confidence that the Dueck suction method is capable of accounting for the water retention behaviour under constant void ratio and in volumetric expansion. However, they do not cover the range of stress conditions that involve volume reduction through consolidation, especially if permanent void ratio changes occur [Gallipoli et al., 2003]. In order to overcome this limitation of the Dueck suction method, the methodology proposed in Chapter 4 is employed for the HM model during consolidation.

5.3 Infiltration Test

The experimental set up for the infiltration test is shown in Figure 5.6. This test was conducted on a 50 mm diameter, 250 mm long bentonite sample compacted to 1.67 Mg/m^3 dry density emplaced in a cylindrical hydration cell [Wang, 2012]. Hydration proceeds from the base of

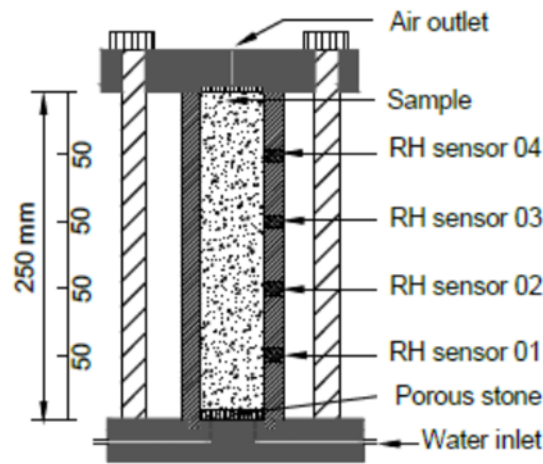


Figure 5.6: Experimental set up for the infiltration test conducted in the SEALEX laboratory tests [Wang, 2012]. Relative humidity sensors are positioned at 50 mm intervals up the sample and hydration proceeds from the base of the cell through a porous stone.

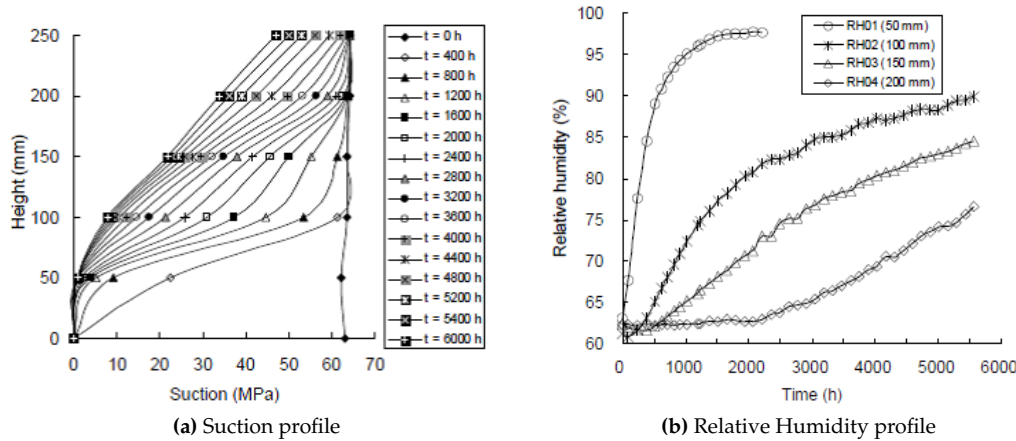


Figure 5.7: Suction profile and relative humidity profile from the infiltration test conducted by Wang [2012] as part of the SEALEX laboratory tests.

the sample through a porous stone and relative humidity is measured at four locations within the sample: 50mm, 100mm, 150mm, and 200mm. Experimentally derived suction and relative humidity profiles for each sensor are presented in Figure 5.7. The relative humidity profile shows a rapid rise to 90% at the sensor located closest to the water inlet (50 mm) in the first c.500 hours, followed by a gradual increase to 98.30% by 1900 hours [Wang, 2012]. The suction profiles show this rapid increase in RH as a decrease in suction at the lowest sensor and a low hydraulic gradient over this interval by the end of the experiment. Sensors 100 mm, 150 mm, and 200 mm show a comparatively gradual increase in relative humidity and a development to a relatively constant hydraulic gradient by the end of the experiment (Figure 5.7(a)).

5.3.1 Conceptual Interpretation of Experimental Results

Wang [2012] interpreted the experimental results with respect to the hydraulic conductivity at each sensor. Hydraulic conductivity was found to be relatively high at high suctions before

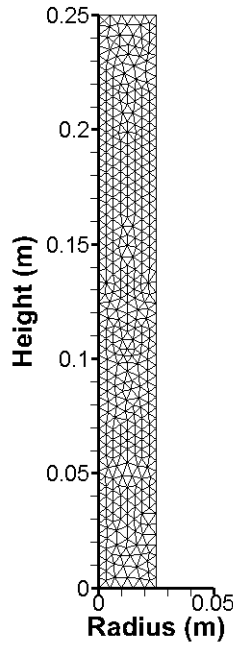


Figure 5.8: The 2D axisymmetric mesh used in the modelling of the infiltration test.

following a ‘U’ shape describing an initial reduction followed by an increase. This could be as a result of deformation during the hydration process; volumetric expansion occurs at the hydration front which initially leads to a consolidation throughout the sample above the base. As hydration proceeds, the porosity and permeability within the sample evolve, leading to a lower permeability at the top of the sample and a higher permeability at the base. This suggests it is important to include a deformation or porosity dependency within the permeability function. To test this, a number of permeability models are tested. Equilibration of suction to the boundary conditions is achieved rapidly at the base of the sample as a result of the increased permeability with expansion. Consequently, the hydraulic gradient is reduced. The following sections describe the modelling method for the infiltration test.

5.3.2 Model set-up

A 2D axisymmetric unstructured mesh of triangular elements was generated using Gmsh [Geuzaine and Remacle, 2009] (Figure 5.8). A hydraulic boundary condition corresponding to liquid water saturation was applied at the base of the sample and zero displacement mechanical boundary conditions were applied to all the model boundaries. Initial conditions were prescribed as the experimental data of suction (from the relative humidity), porosity, void ratio, and dry density. Initial water content was calculated from the water retention curve and the initial suction value. The sample was not considered to be pre-stressed.

5.3.3 Permeability Models

The permeability model used for expansive materials like bentonite will have a significant impact on the accuracy of the solution. In unsaturated soils the effective permeability that

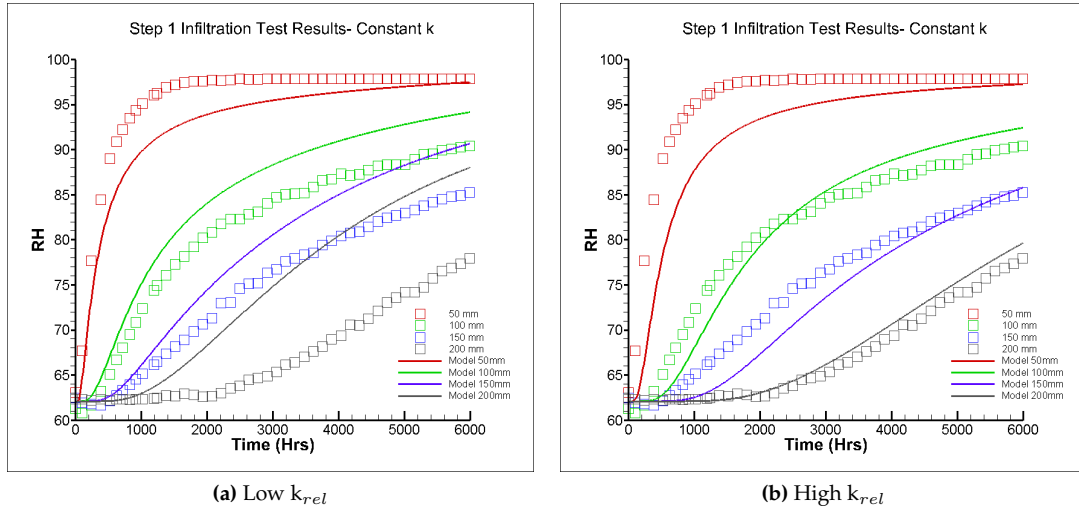


Figure 5.9: Relative humidity calculations using a constant permeability model of $1.5e^{-20}$ and varying relative permeability. It is possible to recreate general trends but the fits to the individual sensors are not good. With a low relative permeability the hydration at the base of the sample is reproduced the best but RH is over predicted in the top of the sample. In the high relative permeability model (S^5) the furthest sensor is well predicted but the initial hydration is under predicted and the shape of the hydration of the middle two sensors is not accurate.

governs the rate of flow is a combination of both the intrinsic permeability and the relative permeability.

5.3.3.1 Intrinsic permeability models

5.3.3.1.1 Constant k

The importance of a permeability model to evolve with deformation of the sample is shown by the model results for a constant permeability model (Figure 5.9). A constant isotropic permeability was considered within the HM framework with deforming mesh and updating porosity, and both intrinsic permeability and relative permeability altered to give the best fit. Figure 5.9 shows the relative humidity calculations for two models (a) and (b) with an intrinsic permeability of $1.5e^{-20}$ and relative permeabilities of $S^{3.8}$ and S^5 respectively (Figure 5.10). The intrinsic permeability value of $1.5e^{-20}$ is on the same order as calculated from the experimentally derived hydraulic conductivity on a similar material by Karnland et al. [2006]. Wang [2012] compared the calculated hydraulic conductivity in the infiltration test for each section between the relative humidity sensors and showed that the infiltration test results have a lower intrinsic permeability than $1.5e^{-20}$ for the majority of sensors over the full suction range.

The model calculations show that a low relative permeability combined with a high intrinsic permeability is needed to begin to reproduce the hydration at the base of the sample, but with a constant intrinsic permeability the relative humidity at the furthest sensors is over-predicted. An increased relative permeability function (S^5) however, reproduces the relative humidity at the furthest sensor well but does not capture the initial hydration at the base of the sample and causes a significant time lag in the hydration of the central sensors. A higher permeability appears to be required to fit the data nearest the water inlet and a lower permeability required to fit the further sensors. Therefore, either the sample does not have a homogeneous

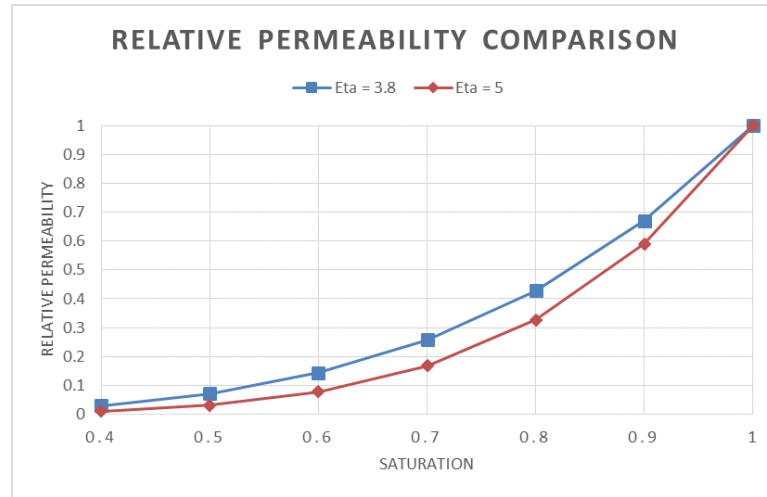


Figure 5.10: The difference in relative permeability for the constant intrinsic permeability model shown over the range of saturations expected in the sample

permeability field (or at least cannot be approximated by a homogeneous permeability field and a function of relative permeability), or the permeability evolves with the change in hydration and subsequent deformation.

A number of permeability models have been proposed for bentonites to take into account their volumetric tendencies, including statistical approaches [Agus, 2005], a model accounting for gel production [Pusch and Yong, 2003], empirical fits to data [Karnland et al., 2006] and variations on the Kozeny-Carmen equation such as the cluster model [Achari et al., 1999] and the 'KC-like' equation [Liu, 2010, Liu et al., 2011, Singh and Wallender, 2008]. These are discussed in Chapter 3 and three models are chosen for comparison here: the in-built KC equation in OGS, the Karnland et al. [2006] empirical formula that is a function of dry density, and the Liu et al. [2011] KC-like equation that is a function of the dry density and the montmorillonite content of the bentonite.

The Kozeny-Carmen equation determines the permeability of a porous medium as a function of the porosity, the specific surface, and the Kozeny constant that reflects the pore-shape and tortuosity of flow channels [Liu, 2010]. Written in terms of volume fraction the K-C equation is repeated here for convenience;

$$k = \frac{1}{k_0 \tau_a^2 a_p^2} \frac{(1 - \phi_k)^3}{\phi_k^2} \quad (5.3)$$

where k_0 is the pore-shape factor, τ_a is the tortuosity of flow paths, a_p is the specific surface area per unit volume of particles, and ϕ_k is the volume fraction of the solid to liquid [Liu, 2010].

The Karnland et al. [2006] empirical model calculates the saturated permeability as a function of the dry density of the sample and is given by

$$k = \alpha_k e^{\beta_k \rho_d} \quad (5.4)$$

where α_k is the permeability at a bentonite dry density of 0 (m^2), β_k is a fitting function, and ρ_d is the bentonite dry density.

The Liu et al. [2011] permeability model is a function of both the dry density of the sample and the montmorillonite content and is repeated again here;

$$k = \frac{\delta_p^2}{4C_k\zeta_p^2} \frac{(1 - \phi_k)^{m_a}}{\phi_k^l} \quad (5.5)$$

where δ_p is the average particle thickness of a montmorillonite sheet (nm), C_k is considered to be the scaled pore shape factor that is a combination of $k_0\tau^2$, ζ_p is the volume fraction of montmorillonite within the solid grains, ϕ_k is the volume fraction of the solid, and m_a and l are calibrating model parameters that determine the dependency of the intrinsic permeability on the solid volume fraction. When m_a and l are equal to 3 and 2 respectively, the function is equivalent to the conventional K-C equation. The volume fraction of the solid is related to the porosity (n) by;

$$\phi_k = 1 - n \quad (5.6)$$

Liu et al. [2011] developed this permeability model for a pure MX-80 bentonite and so the volume fraction (ζ_p) considered the amount of montmorillonite within the bentonite. In the SEALEX experiments the compacted specimen is composed of 70% bentonite and 30% sand and as such, the volume fraction of montmorillonite is further reduced by this ratio. C_k and δ_p are estimated as the average values used in Liu et al. [2011], and m and l are calibrated to the infiltration test results.

5.3.3.2 Relative permeability

Relative permeability is calculated as a power law relationship of the saturation following the method of Brooks and Corey [1964];

$$k_{rel} = S^\eta \quad (5.7)$$

where k_{rel} is the relative permeability, S is the saturation, and η is the power function [Fredlund et al., 2012]. This makes the assumption that the suction value of the partially saturated soil is greater than the air entry suction and reduces to k at full saturation [Fredlund et al., 2012]. As the gas pressure is considered constant for Richards' equation and the modelling only considers the hydration process, the form in equation 5.7 is used to calculate the relative permeability, or coefficient of permeability.

Parameter	Value	Unit	Description	Origin
δ_p	1.2	nm	Ave. montmorillonite thickness	Liu et al. [2011]
C_k	5.0	-	Pore shape factor	Liu et al. [2011]
ζ_p	$0.92M_b$	-	Montmorillonite fraction	Experimental data
m_a	5.5	-	Fitting parameter (Equation 3.38)	Calibrated
l	4.0	-	Fitting parameter (Equation 3.38)	Calibrated
η	3.8	-	Relative permeability power law	Calibrated

Table 5.1: The hydraulic parameterisation of the Liu et al. [2011] permeability function for the bentonite used to fit the infiltration test results. M_b is the mass fraction of bentonite in the bentonite-sand mixture as defined in the experiment [Wang, 2012].

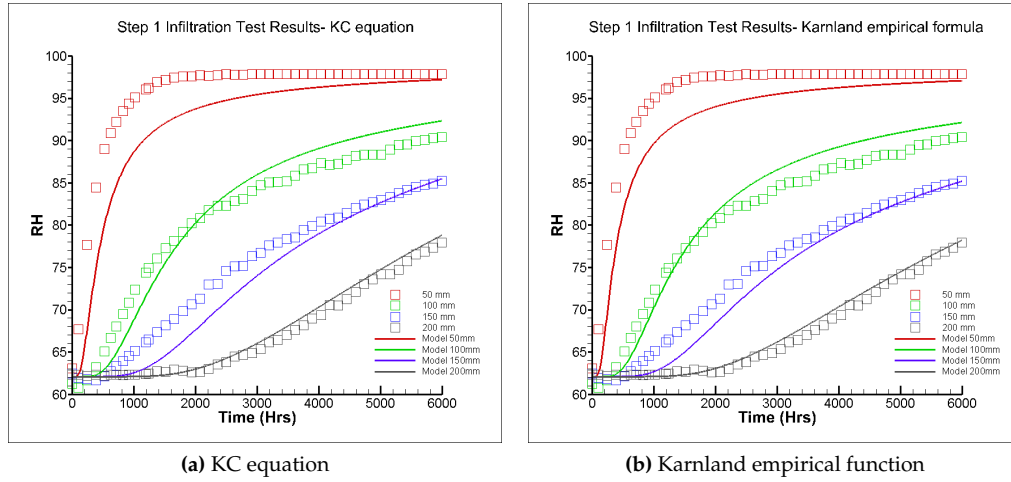


Figure 5.11: A comparison of the in-built KC equation in OpenGeoSys and an empirical formula from Karnland et al. [2006]. The KC equation is unable to match the rapid hydration at the base of the sample and requires a high relative permeability function ($Sr^{4.7}$) to fit the furthest sensors. The Karnland empirical model produces similar results but improves the hydration during the early stages and produces a qualitatively good fit to sensors 100 mm and 200 mm with a lower relative permeability ($Sr^{4.2}$). However, the hydration rate of sensor 150 mm remains under-predicted in the initial stages.

The calibrated relative permeability and intrinsic permeability parameters are shown in Table 5.1

5.3.4 Results

The infiltration test simulations using the in-built KC equation and the Karnland empirical formula are compared in Figure 5.11.

The results indicate that the KC equation is unable to match the rapid hydration at the base of the sample and requires a high relative permeability function ($Sr^{4.7}$) to fit the furthest sensors. The Karnland empirical fit produces similar results but improves the hydration at the base of the sample and produces a qualitatively good fit to sensors 100 mm and 200 mm with a lower relative permeability ($Sr^{4.2}$). However, the hydration rate of sensor 150 mm is not well predicted in the early stages and the fitting parameter β has no clear physical basis.

The results for the infiltration test calculated with the Liu et al. [2011] permeability model are shown in Figure 5.12. A good agreement to the relative humidity profile is achieved, especially for the sensors at 100 mm, 150 mm, and 200 mm. However, although the model nears the final relative humidity value at the end of the test for the sensor closest to the water inlet, the experiment shows a rapid hydration at the base of the sample that the model under predicts. Similarly, when the suction profile is plotted against experimental data the rapid reduction in suction at the base of the sample is under estimated (Figure 5.13).

This is a problem common to all the modelling teams in DECOVALEX-2015 where a fit to the majority of the sensors results in an under prediction in the hydration at the base of the sample. This under- hydration is also evident when comparing the volumetric water content at 400 hrs and 500 hrs with the calculations of Wang [2012] (Figure 5.19). Here the model predicts a higher water content at the top of the sample and at 100 mm than observed (due to a slight deviation from experimental results of the water retention curve fit), but at 50 mm the

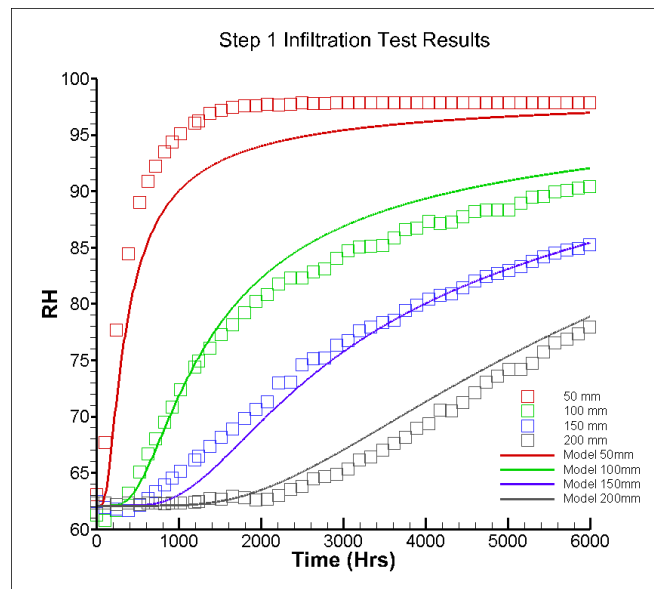


Figure 5.12: Results for the calibrated HM coupled model of the relative humidity profile of the infiltration test.

model under predicts the volumetric water content. This is consistent with the suction and relative humidity data that show that the rapid hydration is not captured by the model.

A comparison of the constant permeability model and the KC-like equation of Liu et al. [2011] is shown in Figure 5.14 where the same relative permeability function is used in both models. The dependence of the permeability on the evolution of the porosity is clearly illustrated by the superior fit to the experimental data produced by the Liu et al. [2011] model, especially the reduction in permeability at the top of the sample due to the hydration and expansion at the base.

Comparisons between the Liu et al. [2011] permeability model and the empirical dry density dependent permeability model of Karnland et al. [2006] show strong similarities. This is to be expected as these both vary as a function of the dry density of the sample. A best fit calibration to the infiltration data show similar capabilities to match the experimental data, although the hydration rate of the lower three sensors is marginally better matched with the Liu et al. [2011] model (Figure 5.15).

In these calibrations the relative permeability function is higher for the Karnland model than the Liu model. Comparing the two models with the same relative permeability function shows a greater difference in the fit to the experimental data between the two models. The results indicate a greater change of the saturated intrinsic permeability for a given change in dry density in the Liu et al. [2011] model as the deformation at the top of the sample leads to a lower permeability and closer fit to the data. This is also shown in Figure 5.16 where the calculated saturated permeability for each model is compared. Over the dry density range expected in the experiment the permeabilities are very similar but the greater dependence of the Liu et al. [2011] model on the permeability at higher dry density leads to the difference in numerical infiltration results. There is no change to the rapid hydration at the base of the sample as the two permeability models are very similar at this dry density (1.67 Mg/m^3 indicated by the green line). However the difference increases with increasing dry density and this

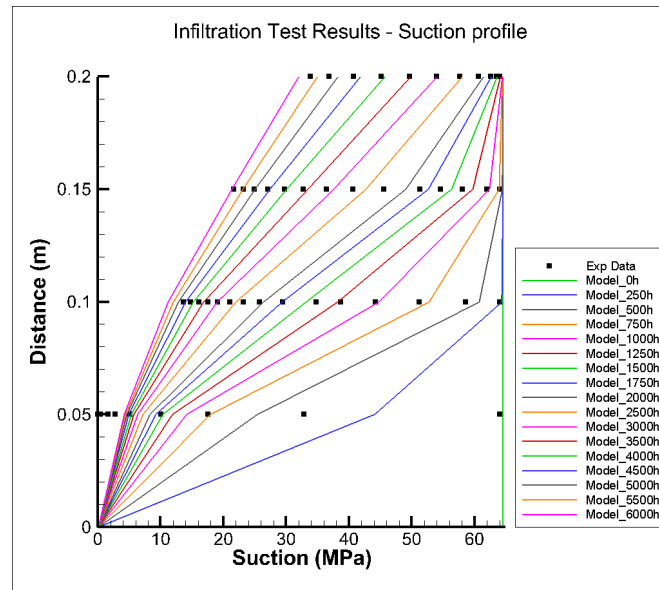


Figure 5.13: Results for the calibrated HM coupled model of the suction profile of the infiltration test.

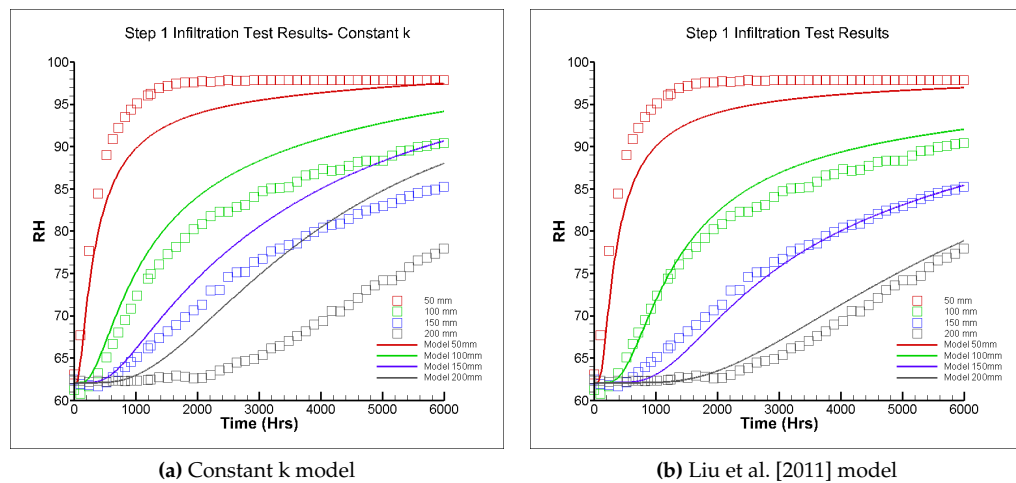


Figure 5.14: A comparison between the infiltration test results achieved with the constant permeability model (a) and the Liu et al. [2011] permeability model (b) . The two models have the same relative permeability function and the difference in fit is attributable to the dependency of saturated permeability on the porosity or dry density of the sample during hydration.

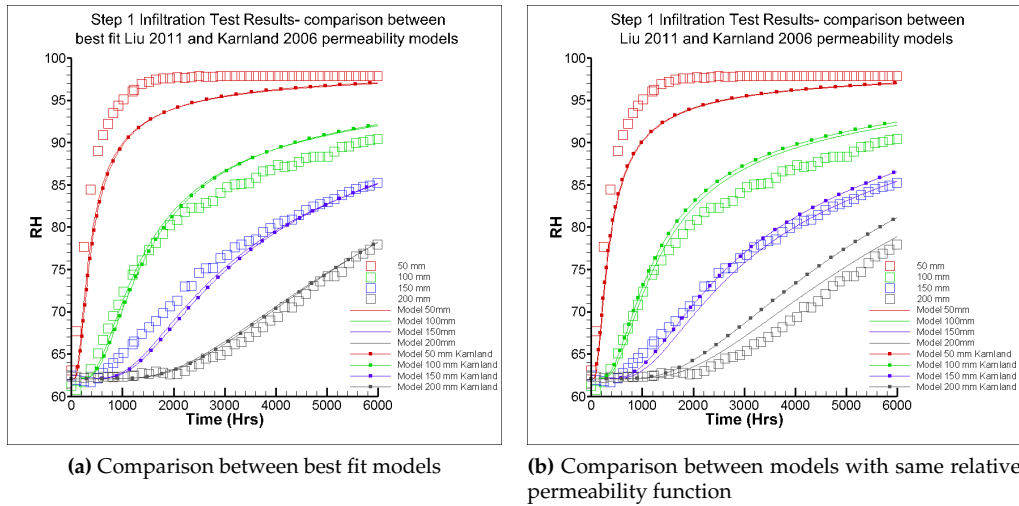


Figure 5.15: A comparison of the best fit results for the Liu et al. [2011] permeability model and the empirical Karnland et al. [2006] model (left). The two models are very similar, although the Liu et al. [2011] model is qualitatively marginally better for the lower three sensors. This is compared to the comparison between the two models with the same relative permeability function (right). The Liu et al. [2011] model is able to better reproduce the experimental data for sensors at 100 mm and 200 mm whereas the Karnland et al. [2006] empirical model has an improved fit to the 150 mm sensor.

leads to a better fit to the experimental infiltration data for the Liu et al. [2011] model. These results indicate that both models are able to reproduce experimental results (except the base hydration) but as the KC-like equation after Liu et al. [2011] has a greater dependency on the dry density of the sample and is not empirically based, it is chosen as the permeability model for the further modelling steps.

5.3.4.1 Evolution of permeability

The change in permeability as a function of constant volume infiltration is shown in Figure 5.17. Initial saturated permeability calculated from the Liu et al. [2011] permeability model is $6.95 \times 10^{-21} \text{ m}^2$ which is lower than that required in the constant permeability model to match the rapid hydration. The initial hydration and expansion of the base of the sample leads to an increase in porosity and permeability close to the water inlet. A maximum permeability of 1.5×10^{-20} is reached at the base of the sample which corresponds to the elevated permeability used in the constant permeability model. The expansion at the base causes consolidation in the top of the sample, which leads to a decrease in porosity and permeability. As the hydrating front travels further up the sample the permeability at the base begins to reduce again, but remains above initial conditions. This is because expansion at the hydrating front causes consolidation at the base. By the end of the hydration test however, saturation has not been reached throughout the sample and the permeability field is not constant; the lower half of the sample has an elevated permeability and the upper half a reduced permeability.

This compares favourably with the calculated hydraulic conductivity by Wang [2012] which reduces further from the water inlet. Assuming a constant water density to convert hydraulic conductivities to intrinsic permeability, the calculated intrinsic permeability at the start of the experiment from Wang [2012] varies depending on the location in the sample (Data dots in

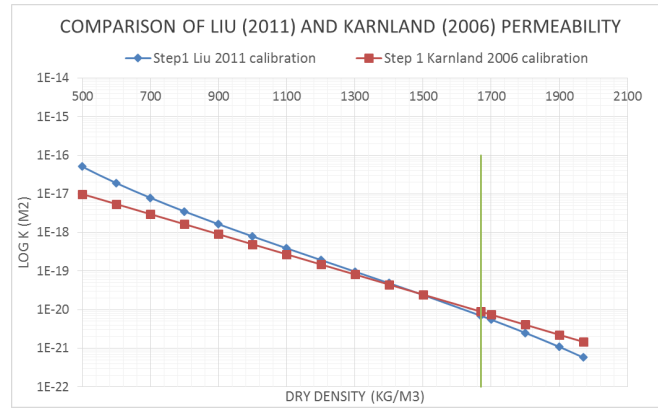


Figure 5.16: A comparison of the saturated permeability calculated across a range of dry densities. The Liu et al. [2011] model shows a greater dependency on the dry density of the sample than the Karnland et al. [2006] empirical function.

Figure 5.18). In the model an isotropic uniform permeability field is assumed at the start of the simulation. A comparison of the calculated permeability in the simulation as a function of the intrinsic and relative permeabilities, and the permeability from Wang [2012] is shown in Figure 5.18. This indicates that the model calculation is in the appropriate range of permeabilities but that the initial permeability is much higher than estimated with the initial conditions. This is consistent with the suction and relative humidity model results which underestimate the rate of hydration at the start of the infiltration test. The shape of the Wang [2012] data suggests a larger reduction in permeability at higher suctions than in the model, which could be caused by a pore clogging mechanism such as gel formation in the pore space [Pusch and Yong, 2003]. The discrepancy between the model permeability and the permeability calculated from the experimental results reflects the inability of the model to account for the rapid hydration at the base of the sample, and the slight over estimation of the relative humidity at the top of the sample. Nevertheless, the model permeability provides a good estimation of the permeability throughout the sample.

5.3.4.2 Water uptake

The comparison in the water uptake of the sample through the duration of the experiment is presented in Figure 5.20. This is calculated via the method suggested in Wang [2012] in which the total volume of water passing each sensor amounts to the total volume of water absorbed by the sample at that time. Here the water uptake is underestimated by a consistent factor. Analysis of the difference in relative humidity between the model and the experimental results can give an indication as to the origin of this underestimation of the volumetric water content. Experimental relative humidity is converted to suction through Kelvin's law (Equation 5.2). The gravimetric water content (M_w) is then calculated from the relationship proposed by Wang [2012];

$$M_w = -7.261 \log(s) + 24.012 \quad (5.8)$$

where s is the suction pressure in MPa and 24.012 corresponds to the maximum gravimetric water content in the experiment [Wang, 2012]. The volumetric water content (Θ) is then

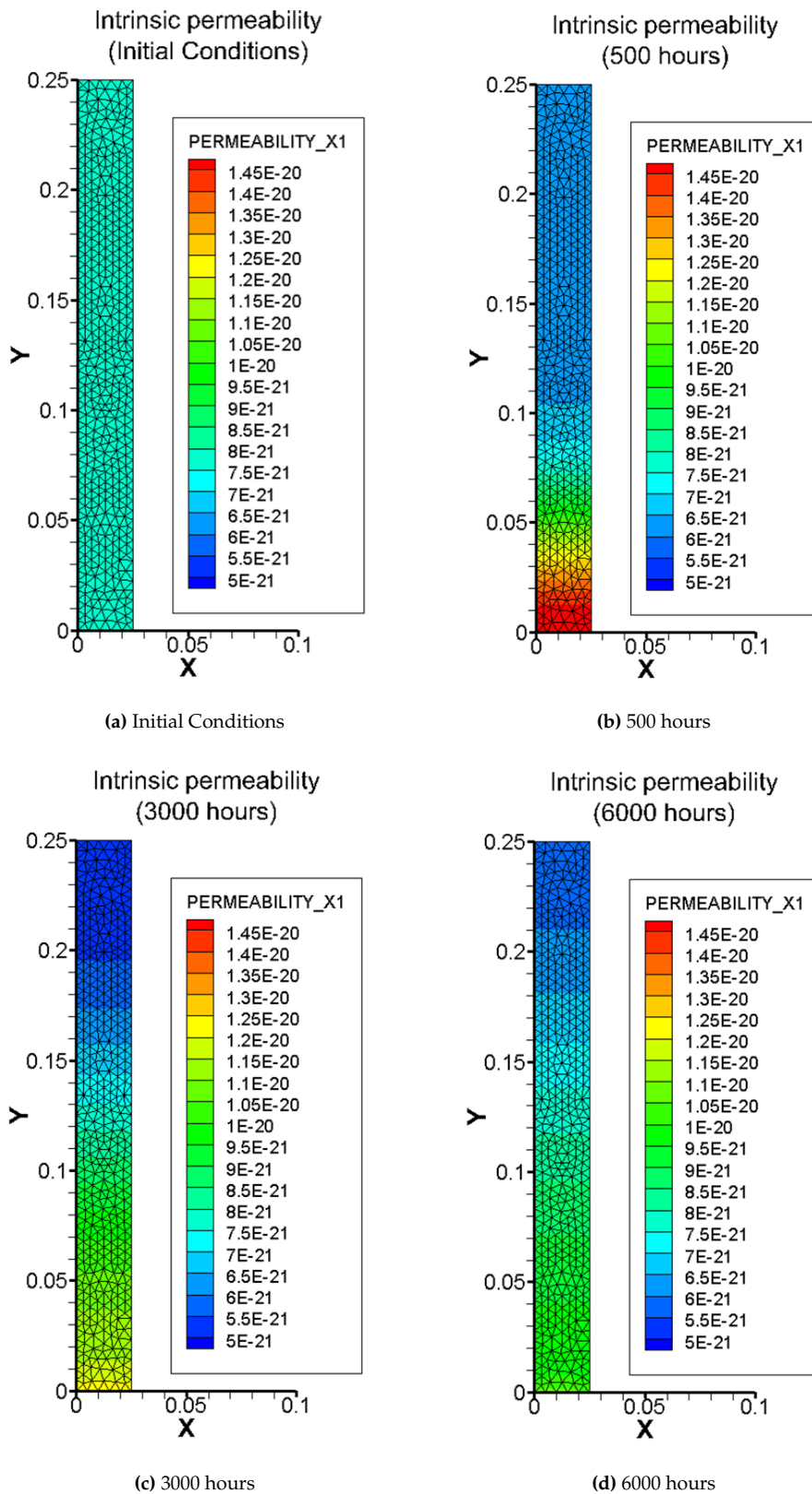


Figure 5.17: The evolution of intrinsic permeability through time in the infiltration test from initial conditions (a) to the end of the simulation (d). The porosity dependent Liu et al. [2011] function calculates an increase in permeability at the base of the sample due to the expansion upon hydration which also causes a reduction in permeability at the top of the sample (b) and (c). As the hydrating front penetrates further up the column the permeability begins to homogenise with a reduction at the base and an increase at the top (d)

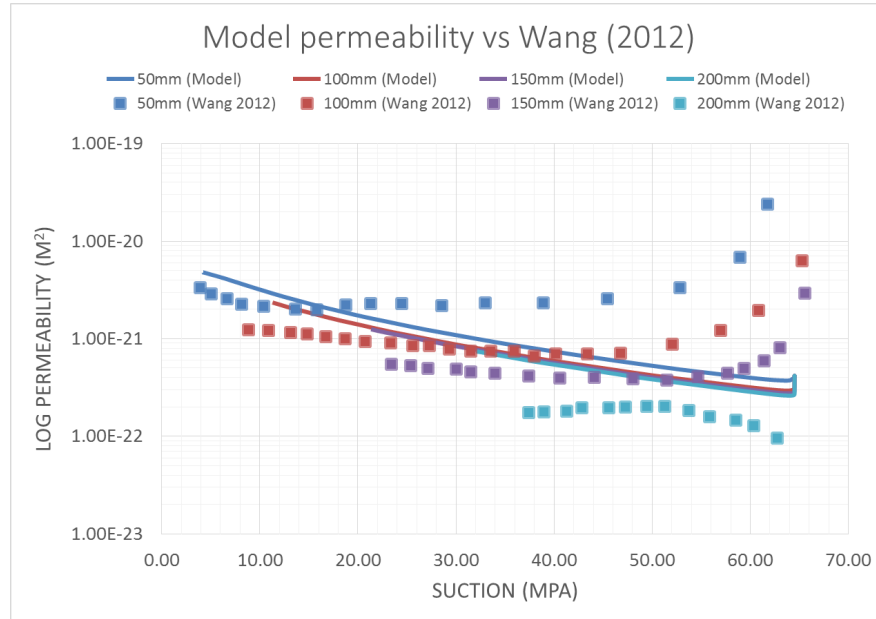


Figure 5.18: A comparison of the model calculated permeability as a function of the intrinsic and relative permeabilities, and the calculated permeability after Wang [2012]. The Wang [2012] calculation shows a higher initial permeability, which may explain the underestimation of initial hydration rate, but the model obtains a good approximation of the permeability at lower suctions.

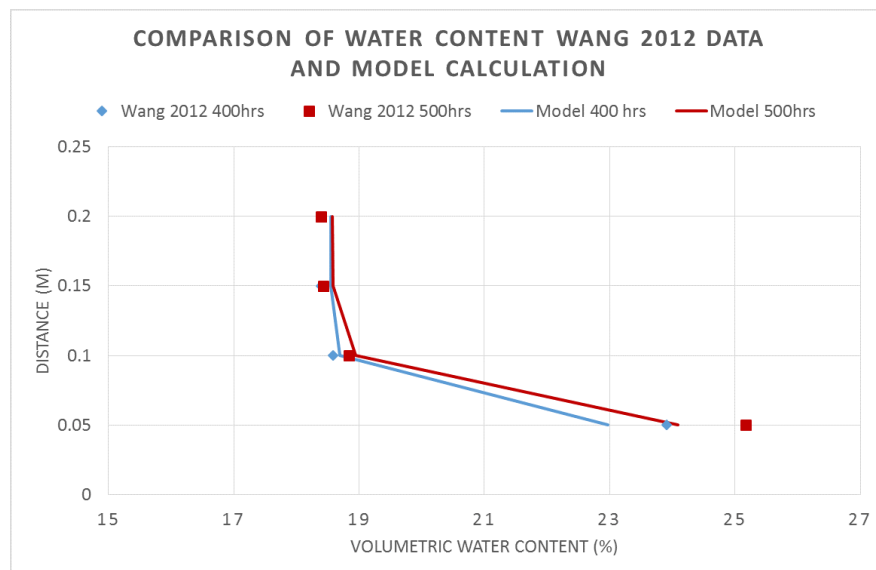


Figure 5.19: Results for the calibrated HM coupled model of the water content after 400 and 500 hrs during the infiltration test. Model results are compared to data from Wang [2012].

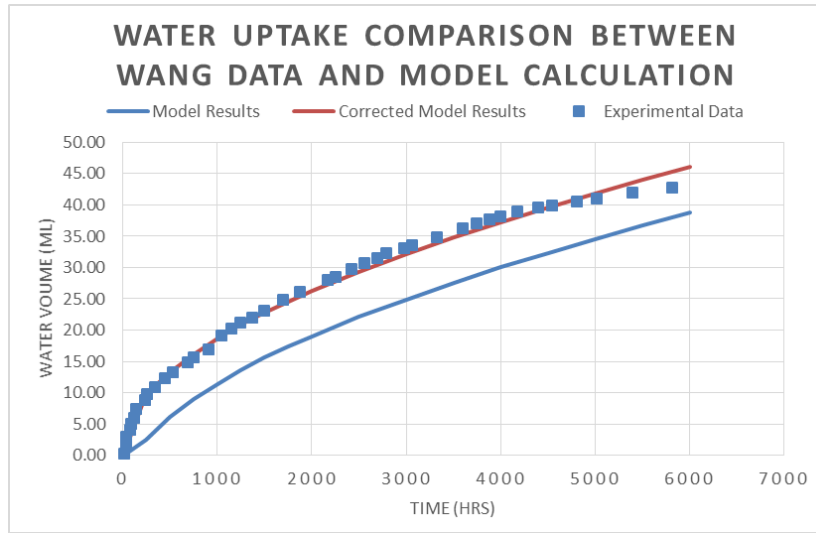


Figure 5.20: A comparison of the calculated water uptake during the infiltration test and the experimental data from Wang [2012]. The model results indicate an under prediction of the water uptake. However, with the consideration of the rapid hydration at the base of the sample the maximum difference in water content between experiment and model corresponds to the difference in water uptake. Applying the maximum difference as a correction factor results in the red line fit of water uptake.

calculated from;

$$\Theta = M_w \left(\frac{\rho_d}{\rho_w} \right) \quad (5.9)$$

where ρ_d is the dry density of the sample considered to be constant for constant volume conditions (kg/m^3), and ρ_w is the density of water (kg/m^3). Applying the above relationship to both the experimental suction and the model calculated suction data reveals that the maximum difference between the calculated and modelled water content at the lowest sensor corresponds to the difference between the calculated water uptake and the experimental water uptake. Both the calculated and a 'corrected' water volume uptake are plotted in Figure 5.20.

The rapid hydration at the base of the sample has been interpreted in view of a separation between the liquid water and water vapour hydration processes. At the base of the sample liquid water causes very fast hydration and expansion of the macro-voids in the sample. As a result the macro-pores become clogged and further hydration continues as a vapour diffusion process [Kröhn, 2003, Wang, 2012, Ye et al., 2009]. Analysis of the pore-structure by Wang [2012] indicates that the evolution of the macro-pores varies at different suctions. For the range of suction from 65 MPa to 12.6 MPa the macro-pores are progressively clogged by exfoliating clay aggregates. However, at low suctions (<4.2 MPa) there is an increase in macro-pore volume because an intermediate pore size evolves as clay aggregates break up [Wang, 2012]. Consequently, the hydraulic conductivity of the sample increases and could explain the high water content and high relative humidity values in the experimental data. The macro-voids are once again clogged as suctions approach saturation (<1 MPa) and therefore inhibit the hydraulic flow of liquid water [Wang, 2012]. Vapour diffusion is then thought to become the dominant process hydrating the rest of the sample [Kröhn, 2003, Wang, 2012].

Nevertheless, even without directly modelling the micro-structure and macro-structure in-

teractions the permeability model implemented simulates an increase in permeability at the base of the sample and an associated decrease in permeability at the top of the sample due to the axial expansion at the hydrating front. With a simple calibration a wide range of dry densities can be modelled, providing a permeability model that can vary with large strain associated with free swelling bentonite. The Liu et al. [2011] permeability model has the greatest dependency on porosity and successfully reproduces the main features of the experimental results (apart from the low suction rapid hydration), and is therefore used in the later modelling steps.

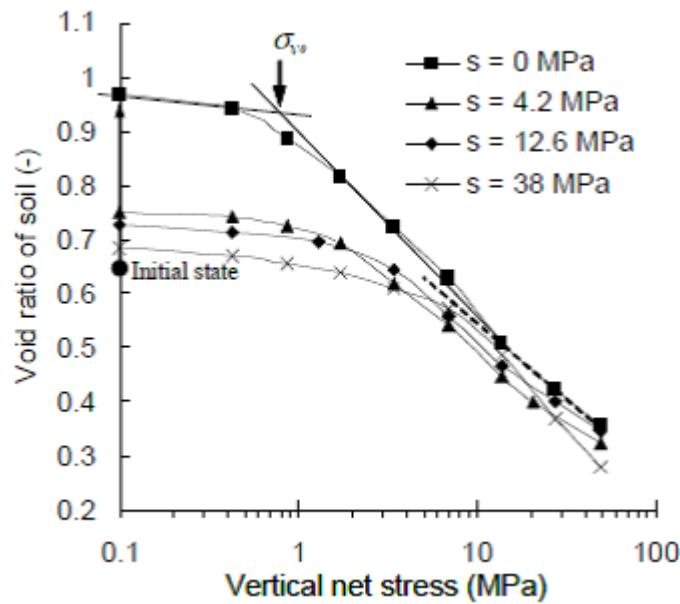


Figure 5.21: Experimental results for the consolidation tests performed on samples of varying imposed suctions [Wang, 2012]. Shown on the figure is the calculation of the pre-consolidation pressure that marks the onset of plastic deformation in traditional elasto-plastic soil mechanics interpretation

5.4 Consolidation Tests

The mechanical behaviour of the bentonite-sand mixture was determined through a series of consolidation tests at four different imposed values of constant suction; 38 MPa, 12.6 MPa, 4.2 MPa, and 0.1 MPa [Wang, 2012]. The tests of the higher suction samples (38 MPa, 12.6 MPa, and 4.2 MPa) were conducted on a 70:30 MX-80 bentonite-sand mixture compacted to a dry density of 1.67 Mg/m^3 and an initial gravimetric water content of 11% Barnichon et al. [2012], Wang [2012]. The lowest suction sample experiment was conducted on the same mixture of MX-80 bentonite and sand but compacted to a dry density of 1.97 Mg/m^3 . Each sample was placed into an oedometer compression cell and allowed to swell to equilibrium with the imposed suction.

The lower density samples were an exact fit to the size of the oedometer ring but the higher density sample had a smaller diameter that aimed to simulate a scaled down technological void. When swelling had stopped the consolidation cycle was started with the load applied from the top. A maximum axial stress of 49 MPa was applied before stress was released gradually and the sample allowed to rebound. Axial strain and applied stress were measured throughout and void ratio calculated to give a standard soil mechanics log stress-void ratio plot for each sample (Figure 5.21). As the hydraulic model is calibrated to the lower dry density samples and the presence of the technological void without radial stress data complicates the hydro-mechanical behaviour of the sample, the mechanical model developed was calibrated to the 1.67 Mg/m^3 density samples.

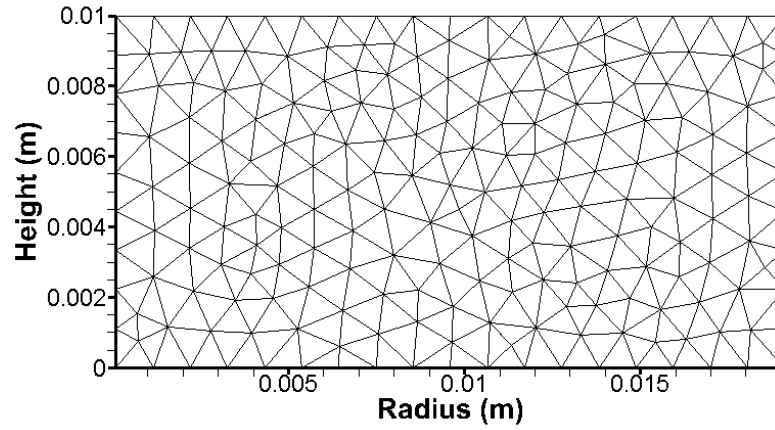


Figure 5.22: The 2-D axisymmetric mesh used for the HM simulation of the consolidation tests.

5.4.1 Conceptual Interpretation of Experimental Results

The experimental results in Figure 5.21 show a non-linear response to the applied stress. As previously discussed in Chapter 2, this response can be considered within either an elasto-plastic or non-linear elastic framework. This thesis is investigating the non-linear elastic interpretation. The consolidation tests conducted at different imposed suctions show differential swelling from the initial state, with larger swelling associated with a lower suction. This results in a variation in pre-consolidation pressure that increases with increasing suction. This observation has been recorded in many soil mechanics studies and is termed suction hardening [Gens, 2010, Nuth and Laloui, 2008]. Nevertheless, the subsequent decrease in volume with increasing stress leads to a convergence of the results towards a common gradient, often termed the virgin consolidation curve [Craig, 2004]. Comparing the 1.67 Mg/m^3 samples, the only factor that causes the variation in the mechanical behaviour is the swelling behaviour to the imposed suction. Swelling leads to a reduction in apparent stiffness, which may be represented by a change in the elastic parameters in a non-linear elastic model. The following sections present the method applied to model the consolidation test results.

5.4.2 Model set-up

An axisymmetric triangular mesh was constructed in the open source mesh generating software Gmsh [Geuzaine and Remacle, 2009]. The moving mesh application requires an axisymmetric implementation because the element volume change is significantly different for radial swelling compared to two-dimensional swelling. This directly effects the element properties in the model such as the dry density, porosity (and therefore permeability in the Liu et al. [2011] model), and mechanical stiffness. The axisymmetric mesh is shown in Figure 5.22 with the axis of rotational symmetry as the left hand edge of the mesh. The mesh for the lower dry density samples has the diameter of the oedometer from the experiments - 38 mm.

Samples were prepared in the same method as the infiltration and water retention tests with a 70:30 bentonite-sand mixture compacted to a dry density of 1.67 Mg/m^3 and initial gravimetric water content of 11% [Wang, 2012]. The initial void ratio was 0.65 and the relative humidity was $c.62.5\%$, which corresponds to an initial suction of 64.5 MPa. There were no

mechanical initial conditions as the sample was in stress equilibrium with the experimental set up.

The hydraulic boundary conditions were the applied suction along the sample base for each consolidation test i.e. 4.2 MPa, 12.6 MPa, and 38 MPa for the lower dry density samples. No flow boundary conditions were applied to the top and sides of the sample. The base and sides were set as zero displacement mechanical boundaries to simulate the oedometer walls, while the top boundary is free to swell in response to the hydration through the sample base.

The mechanical loading of the consolidation test is achieved through a source term. During the suction equilibrium (swelling) stage the mechanical loading is equal to 0.1 MPa i.e. vertical free swelling under the piston. Once the swelling is equilibrated the mechanical load is applied up to a maximum of 49 MPa before being removed to 0.1 MPa. Each timestep during the mechanical loading and unloading cycle is 1 hr. The system is assumed to have equilibrated to the applied load in this time.

5.4.3 Mechanical parameters

The mechanical model as described in Chapter 4 consists of a non-linear function to update the mechanical properties of the sample as a function of the strain history. This function is adapted from that of Dr. habil McDermott for the early stages of DECOVALEX-2015 [Bond et al., 2014] and repeated here for convenience.

$$E_t^{(e)} = E_{t=0}^{(e)} \left(1 + \left(\alpha \sum_{t=1}^{t-1} \Delta \epsilon_{v_t}^{(e)} \right)^d \right) \quad (5.10)$$

where $E_t^{(e)}$ (Pa) is the updated Young's modulus for the given time-step t at element e , $E_{t=0}^{(e)}$ is the initial Young's modulus or reference stiffness (Pa), α is the hardening or softening factor depending on the strain direction (α_h and α_s for hardening or softening respectively), $\sum_{t=1}^t \Delta \epsilon_{v_t}^{(e)}$ is the total volumetric strain the element has seen up to time t , and d is a dimensionality factor. Further to the parameters in the strain-dependent function, the model also requires the input of the Poisson's Ratio (ν) (-), the initial void ratio (-), a threshold elastic modulus (though this is mainly for the large expansive strains seen in Step 2 and Step 3 and is not activated in the consolidation tests) (Pa), the reduction factor (k) (-), and the internal strain factor (γ) (-) as a function of water content. The value of Young's modulus used for each element for each time-step is calculated from;

$$E_t^{(e)} = \begin{cases} E_{t=0}^{(e)} \left(1 + \left(\alpha \sum_{t=1}^{t-1} \Delta \epsilon_{v_t}^{(e)} \right)^d \right) & \text{for } E_t^{(e)} > E_{min} \\ \left(E_{min} \sum_{t=1}^{t-1} \Delta \epsilon_{v_t}^{(e)} \right) \exp^k & \text{for } E_t^{(e)} < E_{min} \end{cases} \quad (5.11)$$

The list of parameters, their units, description and origin are presented in Table 5.2.

The internal strain factor (Υ) is a coupling parameter that is used to define the amount of alleviated suction that translates into skeletal stress (as discussed in Chapter 4). It is varied as a function of the water content to reflect the different hydration processes that predominate at different suctions. At high suctions (low water contents) crystalline swelling controls hydration and bulk volume change. Initially this results in volume change of aggregates being accommodated by the macro-pore space within the bentonite structure before bulk volume

Table 5.2: Mechanical parameters calibrated to the consolidation tests for Step 1 of DECOVALEX-2015 Task A. These parameters are those calibrated for a bentonite:sand mixture with a dry density of 1.67 Mg/m³.

Parameter Symbol	Unit	Description	Origin
E_0	MPa	Initial Young's Modulus	Calibrated
ν	-	Poisson's Ratio	Calibrated
α_h	-	Hardening Parameter	Calibrated
α_s	-	Softening Parameter	Calibrated
d	-	Dimensionality factor	Calibrated
e_0	-	Initial Void Ratio	Experimental data
E_{min}	MPa	Minimum Young's Modulus	Calibrated
k_{red}	-	Reduction factor	Calibrated
Υ	-	Internal Strain Factor	Calibrated

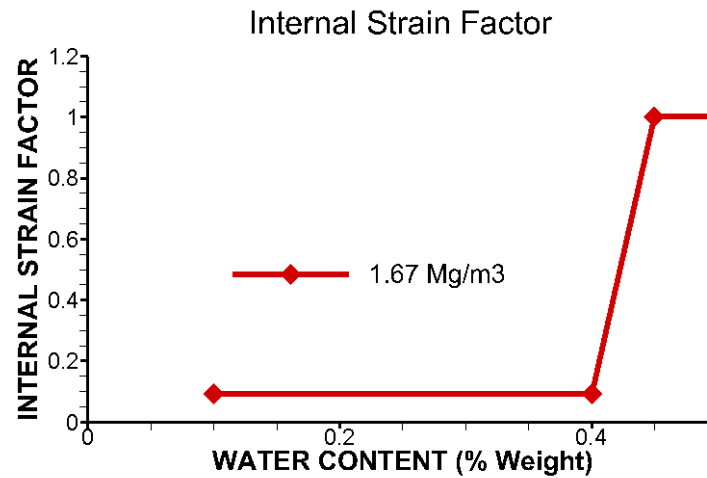


Figure 5.23: The water content dependency of the internal strain factor (γ) used in the coupled HM model for Step 1. The function reflects the difference in swelling processes with crystalline swelling dominant at water contents <40% and osmotic swelling dominant from >40% water content.

change occurs once these pores have been filled. At low suctions (water contents >40% [Waylance, 2008]) the osmotic swelling process dominates and in free swelling conditions leads to massive water uptake and volume change. The water dependency of the internal strain factor is shown in Figure 5.23. The translation of suction change to skeletal stress is low for the crystalline swelling regime but rapidly increases for the osmotic swelling regime.

5.4.4 Results

The mechanical parameterisation and subsequent results presented here are for a fully coupled HM parameterisation. It is possible to achieve good results for all the 1.67 Mg/m³ density samples considering each single test in isolation and a different parameterisation used for each (Figure 5.24). The parameterisation for these consolidation tests is shown in Table 5.3. The mechanical stiffness increases with increasing suction which reflects the increase in pre-consolidation pressure seen in the experimental results. The function in Equation 5.10 is based upon volumetric strain and derived from the consolidation behaviour. Strain caused

Table 5.3: Mechanical parameters calibrated to the consolidation tests for Step 1 of DECOVALEX-2015 Task A. These parameters are varied for each consolidation test to achieve a best fit to each result.

Parameter Symbol	4.2 MPa Suction	12.6 MPa Suction	38 MPa Suction
E_0	30.00	40.00	60.00
ν	0.35	0.35	0.35
α_h	13.00	12.00	7.00
α_s	4.00	4.00	4.00
d	3.00	3.00	3.00
e_0	0.65	0.65	0.65
E_{min}	1.50	1.50	1.50
k_{red}	-1.00	-1.00	-1.00
Υ	$f(wc)$	$f(wc)$	$f(wc)$

by consolidation does not follow the same fundamental process as strain caused by hydration and swelling; the consolidation is driven by external mechanical stress, whereas swelling is driven by the alleviation of suction. As a consequence, the function developed in line with a mechanically driven process does not take into account the change in mechanical properties as a result of varying hydraulic properties i.e. suction, and therefore requires a manual control over the influence of suction on the mechanical stiffness of the bentonite to achieve the best fit to the experimental data.

However, because the consolidation tests on the 1.67 Mg/m³ dry density samples all start with consistent initial conditions, the conceptual model requires that a consistent parameter set is used and the only difference in the consolidation tests be caused by the change in mechanical parameters induced by volumetric swelling to different imposed suctions. Consequently, in the interests of developing a consistent model, a single calibration that provides acceptable results for all the same density samples is required to take forward to the next modelling step.

The consistent parameter set used is shown in Table 5.4. It should be noted that this parameter set does not necessarily represent the best fit that could be achieved for the individual consolidation tests. This is because it was found in later modelling steps that an edit to the mechanical model was required in order to provide an acceptable fit in more complex hydro-mechanical conditions. Therefore, this parameterisation represents the consistent parameter set that is used in all later modelling steps. The experimental results for each sample are shown with the calibrated model results (Figure 5.25).

5.5 Discussion

5.5.1 Hydraulic model

The hydraulic model calibrated to the water retention curve and the infiltration test shows good potential for reproducing experimental data. The permeability model is able to match the general trend of increasing permeability at the base of the sample due to expansion, and decreasing permeability towards the top of the sample. Investigation of the micro-structure by Wang [2012] identified the development of an intermediate structural level of pores that

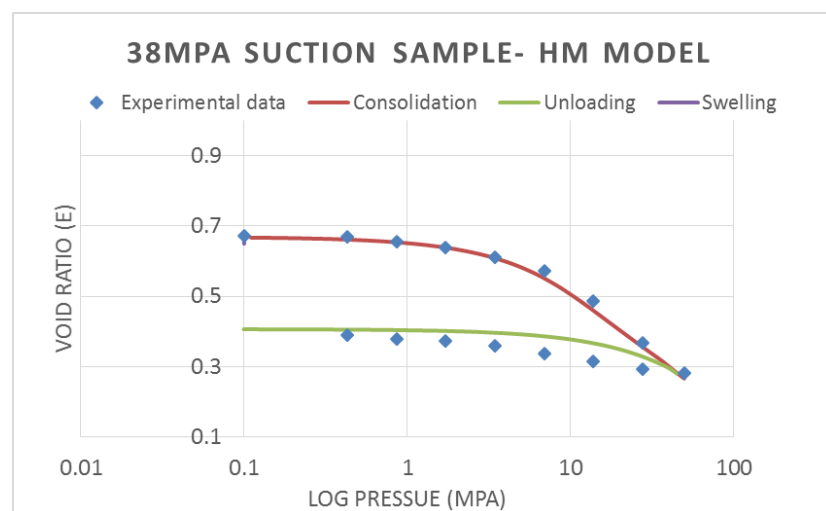
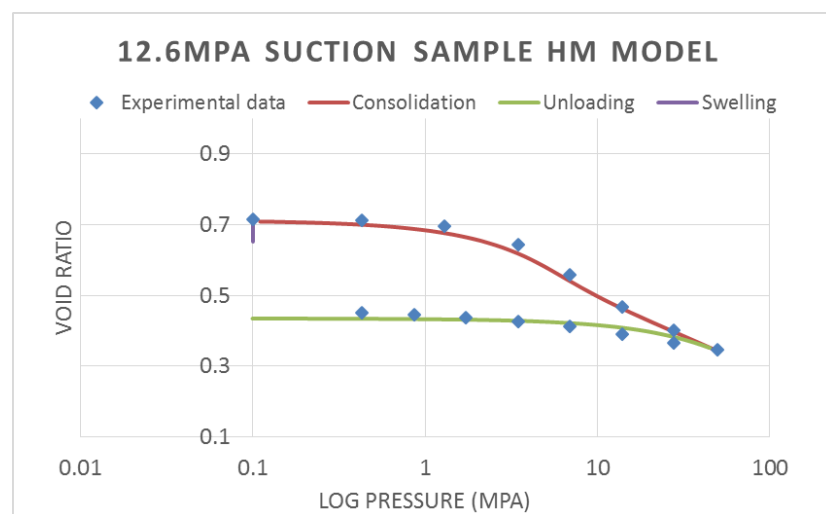
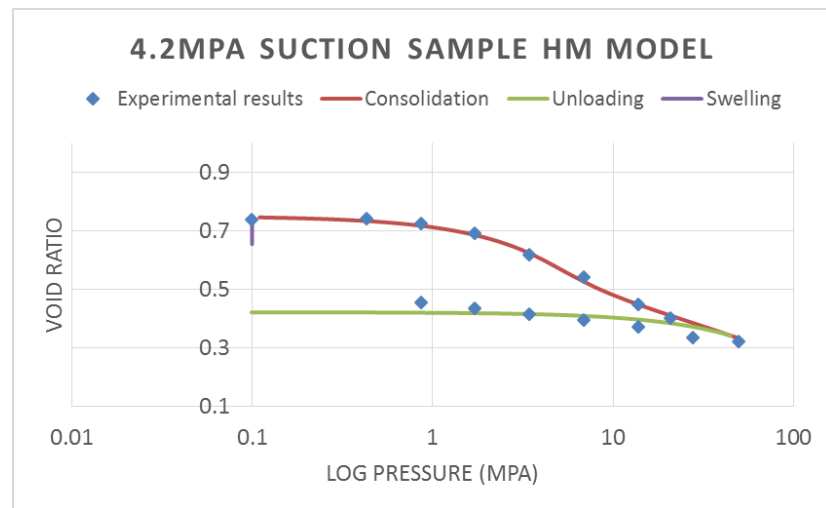
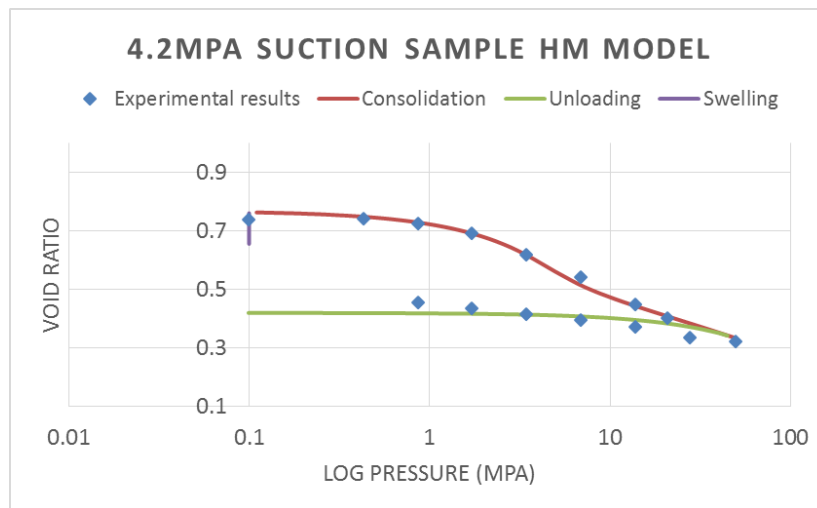
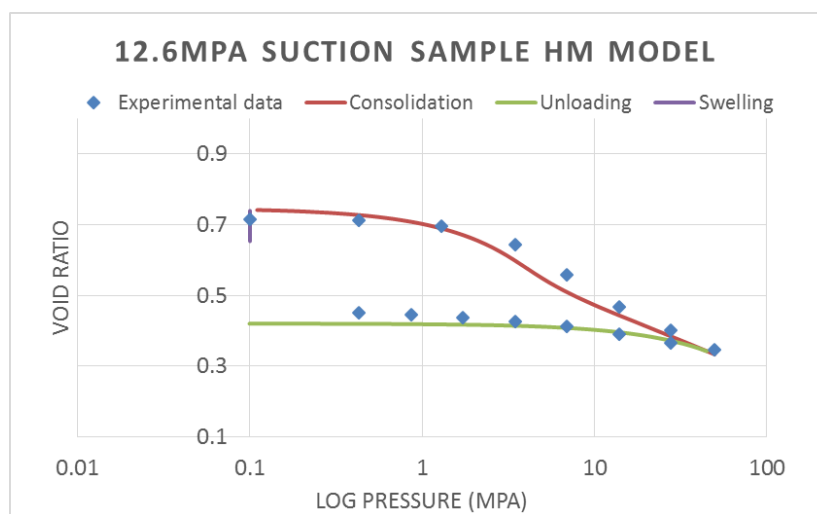


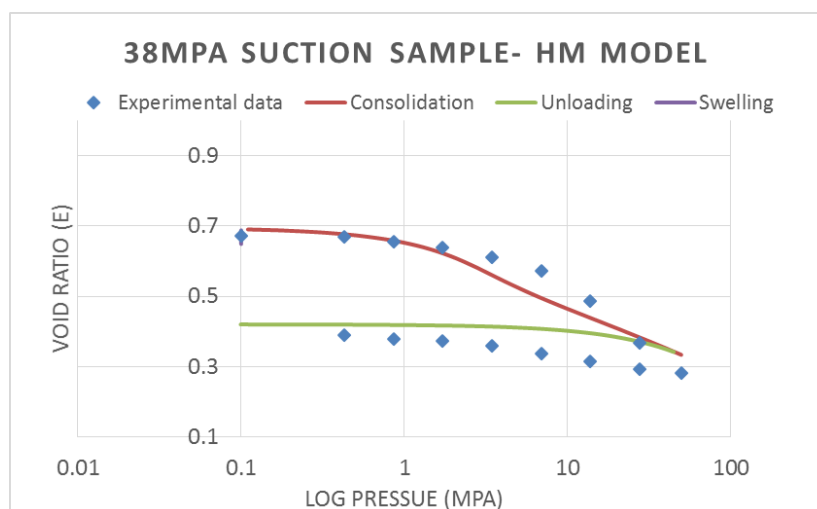
Figure 5.24: The best fit to the lower dry density samples without the technological void achieved by varying the parameterisation between each model. A good fit is achieved in all cases, especially for the initial swelling and consolidation phases.



(a) 4.2 MPa suction sample



(b) 12.6 MPa suction sample



(c) 38 MPa suction sample

Figure 5.25: The consolidation test model results for the samples with a dry density of 1.67 Mg/m^3 . A consistent parameter set is used for each sample that is also used in the later modelling steps. The non-linear elastic formulation is able to recreate the unrecoverable strains seen in the experimental data but does not match well the increase in pre-consolidation pressure with increasing suction.

Table 5.4: Mechanical parameters calibrated to the consolidation tests for Step 1 of DECOVALEX-2015 Task A. These parameters are those calibrated for a bentonite:sand mixture with a dry density of 1.67 Mg/m³.

Parameter Symbol	Value	Unit	Description	Origin
E_0	30.00	MPa	Initial Young's Modulus	Calibrated
ν	0.30	-	Poisson's Ratio	Calibrated
α_h	14.00	-	Hardening Parameter	Calibrated
α_s	3.50	-	Softening Parameter	Calibrated
d	3.00	-	Dimensionality factor	Calibrated
e_0	0.65	-	Initial Void Ratio	Experimental data
E_{min}	1.50	MPa	Minimum Young's Modulus	Calibrated
k_{red}	-1.00	-	Reduction factor	Calibrated
Υ	$f(wc)$	-	Internal Strain Factor	Calibrated

develop at low suctions before becoming clogged and interpreted the rapid hydration of the lowest sensor to be as a result of the break-up of sodium montmorillonite aggregates resulting in increased permeability. In order to characterise and model this micro-macro structure evolution a model would need to explicitly address the structural levels and their interactions, which would also require parameterisation of individual water retention curves for each structural scale [Alonso et al., 2011, Gens et al., 2011, Navarro et al., 2015]. However, the model developed here does not consider the individual structural levels deliberately in order to maintain a simple parameterisation. Therefore, to test the applicability of the developed and calibrated model for infiltration tests and to determine if the structural scales need addressing explicitly, the model was applied to another data set on the GMZ bentonite in Ye et al. [2009].

The GMZ bentonite is also a sodium bentonite but has a higher calcium and magnesium content than MX-80 [Ye et al., 2009]. The infiltration test results were obtained for a 150 mm long, 25 mm wide cylindrical sample compacted to a dry density of 1.70Mg/m³. The bentonite was not mixed with sand but the montmorillonite content was 75% in contrast to 92% in the MX-80 bentonite. A similar experimental set up was used for infiltration, and relative humidity data was recorded at 5 locations at 30 mm spacing. The permeability model has the parameters to take the physical differences in bentonites into account and can approximate the difference in cation composition through the m and l parameters. The free swell water retention curve was calibrated to the experimental free swell water retention data and the results are presented in Figure 5.26.

The same mechanical model that was used for the MX-80 bentonite (and parameterised in the previous section) was used as a first approximation to test the applicability of the hydraulic model. The water retention data showed some interesting features that do not quite fit with the conceptual model e.g. the constant volume water retention data showed a higher water content for a given suction at high suctions in comparison to the free swell data, and the initial conditions for the infiltration test of 12.3% gravimetric water content did not correspond with an initial suction of 80 MPa as described in Ye et al. [2009]. A suction of 80 MPa corresponds to c.15-16% gravimetric water content in the water retention test data, but in an effort to conform to the initial conditions of the experiment a best fit line through the scattered data points and

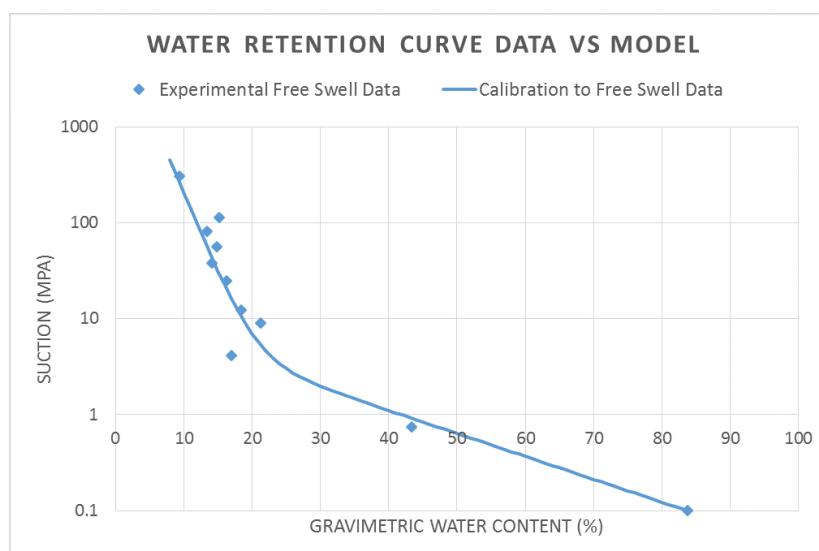


Figure 5.26: A graph showing the calibration to the free swell water retention data obtained by Ye et al. [2009] on the GMZ bentonite. The calibrated curve is used as input for the hydraulic model.

as close to the 80 MPa suction - 12.3% water content restraint as possible was used.

Even though the water retention curve is a sensitive parameter in an unsaturated hydraulic model and could potentially be a source of error, the applicability of the model is seen in Figure 5.27 with the parameterisation shown in Table 5.5. An excellent fit to the initial hydration of all five sensors is achieved. The application of the chosen model to this separate bentonite gives confidence that the model is reproducing the main processes in the experiments, and can therefore be used in future modelling steps.

It also allows a degree of interpretation to be made when the model prediction deviates from the experimental results. Final relative humidity is well matched in all sensors except the sensor closest to the water inlet which shows a stepped increase in relative humidity after c.2000 hrs. Interpretation of this behaviour in view of the conceptual model provided by Ye et al. [2009] and Wang [2012], suggests that the difference in interlayer cation from predominantly Na^+ to a mixture of Na^+ , Ca^{2+} and Mg^{2+} , could lead to a different temporal evolution of the micro- and macro-structures. The greater charge of the Ca^{2+} and Mg^{2+} cations in the interlayer cause initial hydration to be accommodated by particles with this counterion. Bentonites with calcium as the dominant cation have less propensity to exfoliate [Likos and Lu, 2006, Pusch et al., 1990], and as such the initial hydration may not lead to the same development of intermediate macro-pores at the beginning of hydration as seen in the MX-80 bentonite in the SEALEX experiments. The later step in relative humidity could represent the development of these intermediate macro-pores at low suctions and an increase in hydraulic conductivity [Wang, 2012] when hydration of the Na^+ dominated aggregates becomes dominant and causes them to break up.

The ability of the permeability model to be adjusted for the different mixture compositions of bentonites and reproduce experimental results with only a minor change in parameterisation lends confidence in the hydraulic model for use in more complicated hydro-mechanical conditions.

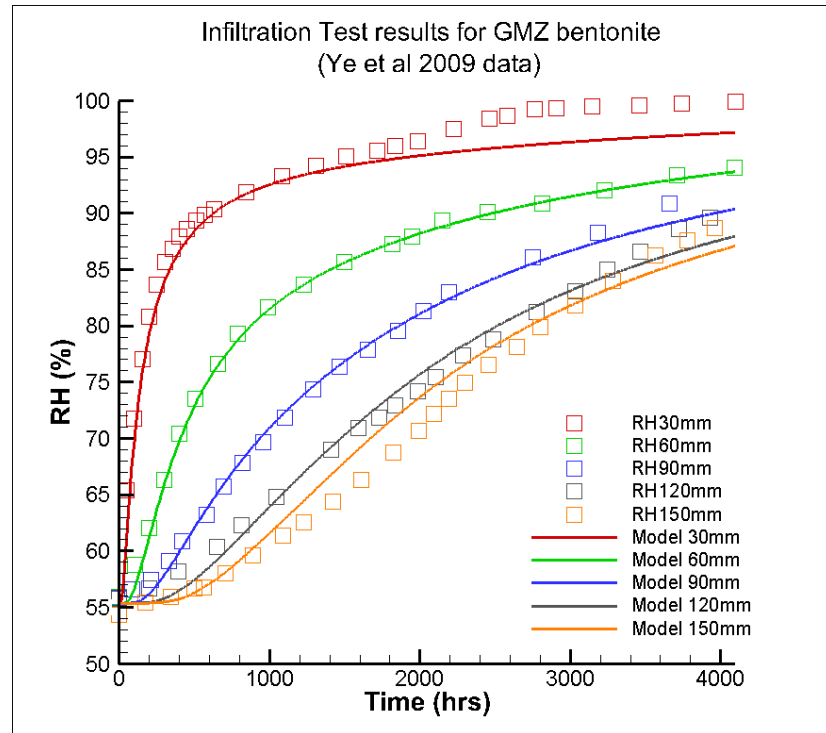


Figure 5.27: Relative humidity results calculated from the infiltration test on GMZ bentonite by Ye et al. [2009]. An excellent fit is achieved after taking into account the differences in bentonite used with only a minimal change in fitting parameters (see Table 5.5). This provides confidence in the applicability of the hydraulic model.

Parameter	Value	Unit	Description	Origin
δ_p	1.2	nm	Ave. montmorillonite thickness	Liu et al. [2011]
C_k	5.0	-	Pore shape factor	Liu et al. [2011]
ζ_p	$0.75M_b$	-	Montmorillonite fraction	Experimental data
m	5.2	-	Fitting parameter (Equation 3.38)	Calibrated
l	4.0	-	Fitting parameter (Equation 3.38)	Calibrated
η	3.8	-	Relative permeability power law	Calibrated

Table 5.5: The hydraulic parameterisation of the Liu et al. [2011] permeability function for the GMZ bentonite in Ye et al. [2009]. The experimental mass fraction of montmorillonite was adjusted and the m parameter changed from 5.5 to 5.3 in order to fit the infiltration test results. M_b is the mass fraction of bentonite which is equal to 1 in the Ye et al. [2009] experiments.

5.5.2 Non-linear elastic model

The non-linear elastic model is able to reproduce the unrecoverable strains observed in the consolidation test results. A best fit calibration to each test at different imposed suctions enables a good fit to the data and provides encouragement that the non-linear elastic approach can model the behaviour with only 4 parameters. However, as the tests started from the same initial conditions, a consistent HM parameterisation is required. The mechanical model is developed as a function of the strain of the sample and therefore considers the hydraulic affect on the mechanical properties to be a function of the volume change caused by the change in suction. This provides an indirect coupling between the mechanical properties (mechanical stiffness) and hydraulic properties (suction). In elasto-plastic models such as the BBM [Alonso et al., 1999] the modified Cam Clay model, in which the failure criterion is formulated in terms of net mean stress and deviatoric stress, the mechanical model is extended to include a dependency on suction. This current work does not include this dependency on suction directly but couples the mechanical properties with the hydraulic properties through the volume change.

The mechanical model was developed based primarily on the consolidation phase of the consolidation tests. As the experimental samples had consistent and comparable initial conditions, the implication of the results indicating that the increase in pre-consolidation pressure is not well matched is that the dependency of the mechanical stiffness on suction during swelling requires further development. Future work on the mechanical model for the consolidation tests using the same framework should consider the fact that a reduction in suction may cause both a hydraulic stress acting on the mechanical skeleton of the sample, and also a reduction in stiffness. Analysis of the best fit calibrated values of E_0 indicate an empirical relationship that could be used for future development of the mechanical expansive model. This relationship is shown in Figure 5.28 and indicates that an initial Young's modulus common to the three tests is between 63.287 MPa and 66.838 MPa depending on the method of extrapolation (polynomial or linear respectively). Using this relationship the value of E_0 in the mechanical model could be varied as a function of the strain. Furthermore a relationship can be determined from the best fit models between the hardening parameter and the strain (Figure 5.29) that could be used in conjunction with the calculation of the E_0 function to define the mechanical conditions at the start of the consolidation phase. Although the implementation of this dependency of the mechanical stiffness on the suction and strain would be an empirical extension of an empirical formula to improve the swelling model, it could provide a methodology for determining parameters of future models.

This methodology allows the best fit consolidation test models to define an axial swelling model for samples compacted to a dry density of 1.67 Mg/m^3 and hydrated to a suction of 4.2 MPa.

5.5.2.1 HM implications of consolidation tests

The consolidation tests can be further analysed in terms of the hydro-mechanical behaviour by investigating the net axial stress at which saturation is calculated to occur. Wang [2012] determined saturation points for each of the low dry density samples. In order to do this, Wang [2012] used an estimation of the water content at the point of full hydration to the imposed suctions. This was determined from a water retention curve re-formulated to be in terms of water volume ratio and suction pressure [Wang, 2012]. However, the calculated water con-

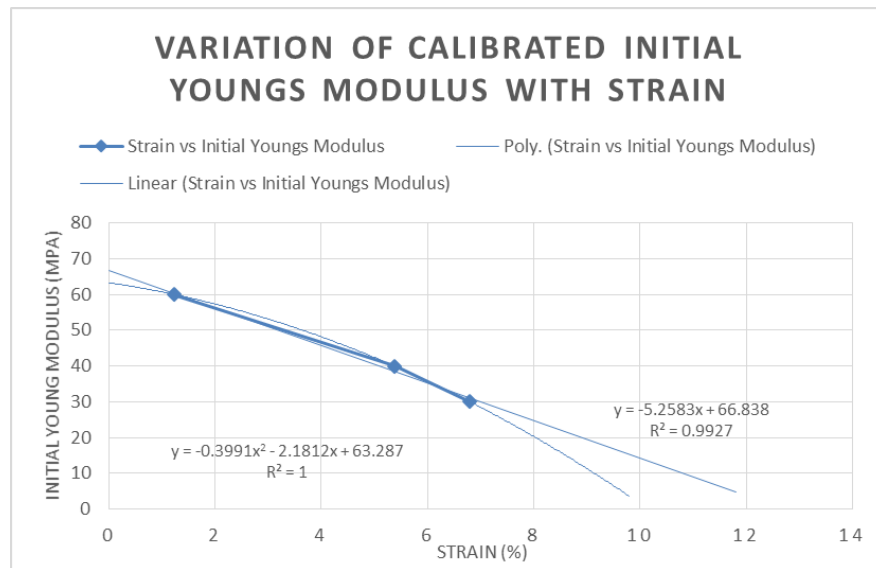


Figure 5.28: The variation of calibrated initial Young's modulus with experimental strain in the low density consolidation tests during hydration to the imposed suction. Applying a linear or exponential fit to the data indicates a starting Young's Modulus of between 63 and 67 MPa.

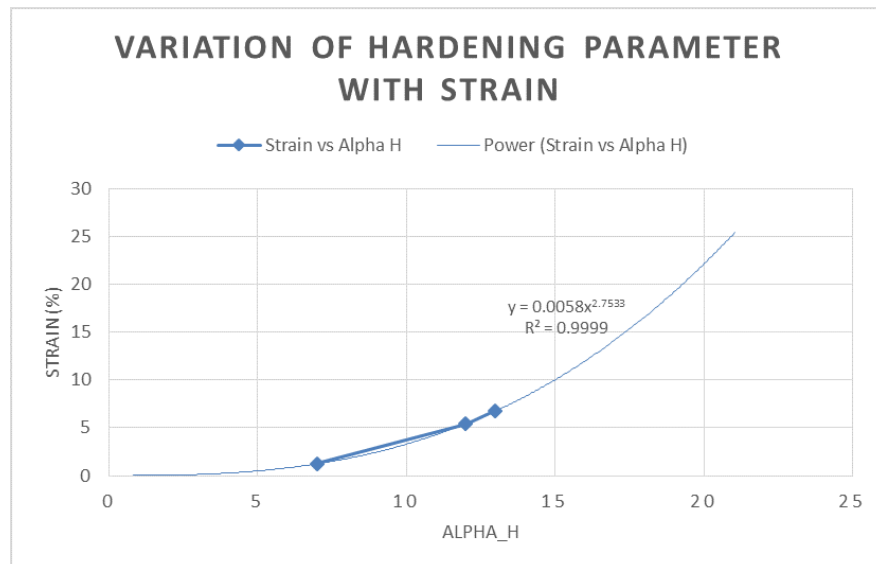


Figure 5.29: The variation of calibrated hardening parameter (α_h) with experimental strain in the low density consolidation tests.

tent values correspond closely to the water retention curve derived for constant volume even though there is volumetric expansion during hydration to the imposed suctions. Nevertheless, Wang [2012] interpreted the saturation points to correspond with the inflection points of the consolidation test results and inferred that this change in hydro-mechanical behaviour was due to the unsaturated macro-pores becoming fully destroyed and the subsequent change in volume with stress determined by the deformation of the aggregates.

The model results were investigated to see if the saturation points could be predicted and the plot is shown in Figure 5.30. The model predicts a higher initial saturation point for the lower suction samples as a higher water content is determined from the Dueck suction defined partially confined water retention curve. This is due to the discrepancy in hydrated water content assumption between that of the calculation in Wang [2012] and the Dueck suction water retention curve (Figure 5.19), and implies the sensitivity of hydro-mechanically coupled models to the method of calculating the water retention curve for different stress conditions. However, the shape of the change in saturation with increasing net axial stress corresponds well to that of the calculated data in Wang [2012] for the lower suctions. The 38 MPa suction case does not fit the saturation point data and, in fact, does not reach saturation at any point. This is due to the larger discrepancy in the change in void ratio with net axial stress seen in the consolidation test model (Figure 5.25). As the model calculation does not recreate the same magnitude of void ratio change the point of saturation is not reached. Figure 5.30 also shows the saturation point fit achieved with the best fit parameterisation of the 38 MPa sample shown in Table 5.3, which is greatly improved. At 38 MPa suction the constant volume and free swell water retention curves are closest and, as such, the good fit achieved by the model to both the mechanical and hydraulic behaviour at this suction indicates that the simple formulation is capable of accurately reproducing the hydro-mechanical behaviour for individual tests. However, as previously mentioned, the dependency of mechanical properties on hydraulic conditions (i.e. suction) is not directly accounted for in the non-linear elastic formula and, as such, a consistent model parameterisation is not able to fully recreate all aspects of the consolidation tests behaviour.

5.6 Conclusions

A non-linear elastic mechanical model coupled to a Richards' model for unsaturated fluid flow has been calibrated to a series of laboratory experiments to provide a fully coupled HM numerical modelling tool. The model requires input in the form of the free swell water retention curve and experimentally derived properties of the medium, such as dry density, void ratio, and porosity. The hydraulic model is parameterised by 4 parameters for intrinsic permeability, and 1 parameter for relative permeability. The mechanical model requires 8 parameters to describe both swelling and consolidation, of which, 7 are calibrated and 1 is experimental initial conditions, and a further coupling parameter is introduced. In total, the model requires 10 parameters to provide a good agreement to experimental results for a range of hydro-mechanical conditions from swelling, constant volume infiltration, and consolidation. This is fewer than models such as the Barcelona Expansive Model (BExM), which requires 14 mechanical parameters to calculate the mechanical behaviour of a constant volume swelling test [Navarro et al., 2015].

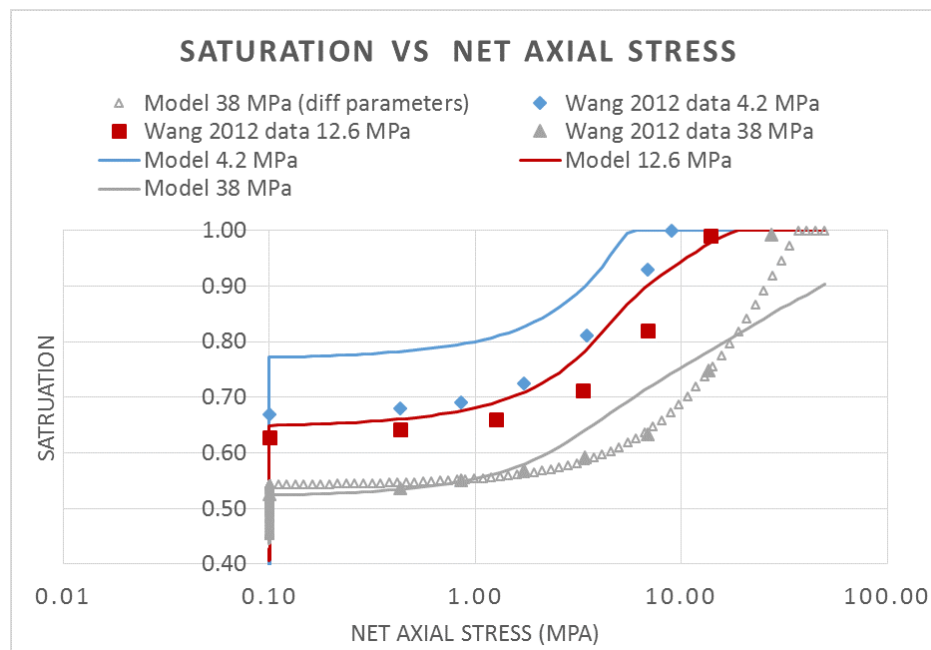


Figure 5.30: Model predictions of the change in saturation with increasing net axial stress in the consolidation tests on 1.67 Mg/m^3 samples using the consistent parameter set (lines). Also shown is the model prediction for the 38 MPa sample when the consolidation behaviour is more accurately fitted (than in the consistent parameter set model) (open triangles).

Chapter 6

Modelling Step 2 of the SEALEX experiments

In this Chapter the non-linear elastic model is applied to a 1:10th scale mock-up test of a hydraulic seal. Displacement dependent boundary conditions making use of the Lagrangian moving mesh are developed to simulate the technological void. A novel approach is presented as an extension to the non-linear elastic model to account for wetting-induced collapse behaviour observed in experiment. A failure curve based on experimental data is defined that activates a source term to reduce axial stress build up. This approach is compared to the non-linear elastic results and discussed with respect to elasto-plastic model formulations.

6.1 Introduction

The laboratory experiment used for the Step 2 modelling task was a 1:10 scale mock-up of the SEALEX *in situ* test. The experimental set-up is shown in Figure 6.1 and comprises a 55 mm diameter by 120 mm height compacted bentonite-sand mixture sample at a dry density of 1.97 Mg/m³. The same ratio of 70% bentonite to 30% sand was used in the mixture. The sample was placed in the centre of a rigid hydration cell with a diameter of 60 mm to produce a symmetrical technological void around the sample. The cell was able to hydrate through porous stones at both the base and the top of the sample [Wang, 2012]. A piston 60 mm in diameter and 150 mm long acted at the top of the sample to control the axial deformation through the different phases of the experiment.

Step 2 was divided into three main phases (Figure 6.2):

- Phase 1: The Initial Saturation Phase [Wang, 2012] consisted of flooding of the technological void with subsequent hydration from both the void and the base of the sample. During this phase axial deformation was restrained and the build-up of axial stress was measured. The injected water volume was also measured.
- Phase 2: The Void Recovery Phase [Wang, 2012] was initiated after axial stress equilibrium and involved the removal of the confining axial pressure. This phase was further subdivided into:
 - Phase 2a: Hydration through the sample base only, and

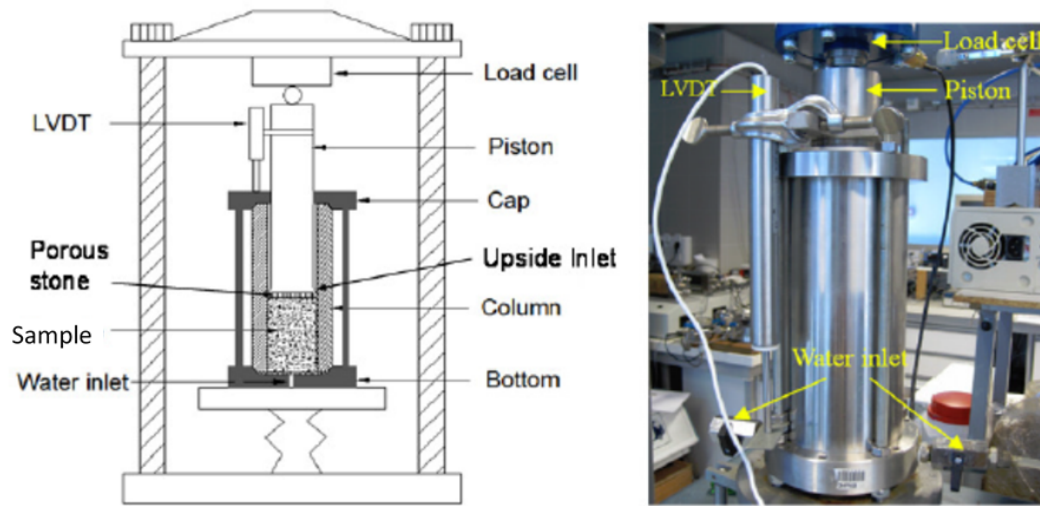


Figure 6.1: A schematic diagram and image of the experimental set up for the Step 2 mock-up test [Wang, 2012].

- Phase 2b: Hydration from the base and the top simultaneously [Wang, 2012].
- Phase 3: The Confinement Phase was activated after 20% axial strain during Phase 2 as the piston was clamped to prevent further strain, and the axial stress build up was measured.

6.2 Conceptual Interpretation of Experimental Results

The results are presented for the axial stress evolution throughout the experiment, the water uptake during the Initial Saturation Phase, and the displacement during phase the Void Recovery Phase.

6.2.1 Axial Stress

The axial stress evolution through the experiment is shown in Figure 6.3 and annotated to show the three phases. During Phase 1 there is an initial peak at *c.*12 days, followed by a reduction until *c.*30 days, before a build-up in axial stress and plateau after 250-260 days. This evolution of axial stress is closely matched by the evolution of axial strain, as shown in Figure 6.4 [Wang, 2012]. The physical process occurring during the reduction in axial stress has been interpreted as a wetting-induced collapse phenomenon [Wang, 2012], and has been observed in other experimental programmes during hydration of bentonite [Gens et al., 2011, Lloret et al., 2003, Romero et al., 2003, Saba, 2014]. A number of hypotheses have been suggested for this phenomenon based on the collapse of the macro-structure in the double structure concept of bentonite pore space [Agus, 2005];

- Breaking of cementing bonds between grains in initially dry samples as the water hydrates the pore space,

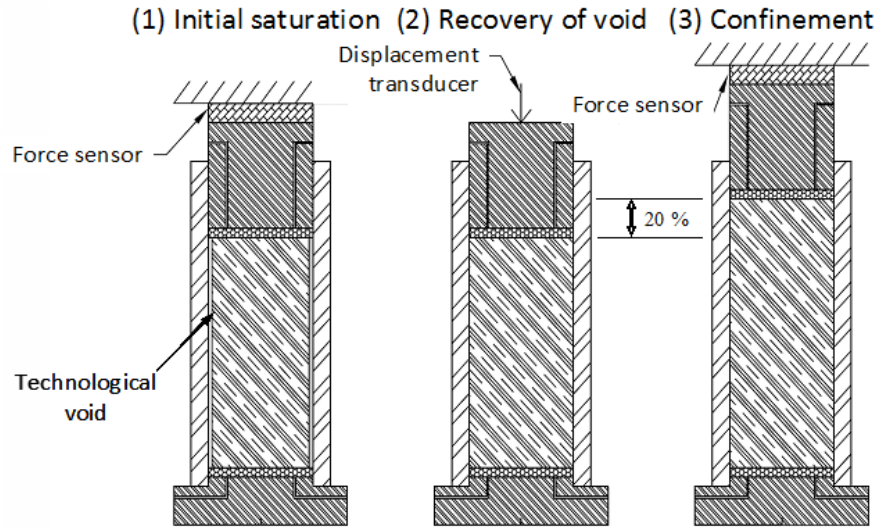


Figure 6.2: A schematic diagram illustrating the three phases of the Step 2 mock-up test [Wang, 2012].

- Structural rearrangement of clay clusters within the sample as a result of the frictional coefficient of the soil being overcome by wetting-induced shear forces at the micro-scale, or
- Collapse of the macro-structure in response to the developed swelling pressure/confining load [Lloret et al., 2003]

Experimental constant volume conditions are maintained by an increase or decrease in applied load in response to axial strain [Lloret et al., 2003, Wang, 2012]. The reduction in axial stress during experiments is measured when the collapse phenomenon occurs and the experimental equipment varies the axial load acting on the sample. This is evidenced by the measurement of strain at the sample top during the initial hydration phase of the Step 2 mock-up test (Figure 6.4) [Wang, 2012]. The axial strain follows closely the shape of the axial stress measurements indicating that a physical collapse is responsible for the reduction in the axial stress. This can also be interpreted as macro-structural compressive strains which are partially offset by expansion of the micro-structure [Lloret et al., 2003]. In order to model the axial stress development during Phase 1 the non-linear elastic model needs to account for the macro-structural compressive behaviour.

During the Void Recovery Phase (P2 on Figure 6.3), there is no compressive axial stress as the sample expands to fill the void. The Confinement Phase (P3 on Figure 6.3) shows a further build up in axial stress. The rate of this axial stress development is lower than the initial saturation phase, but builds up until a plateau at the c.500 day mark. This suggests that the sample maintains a suction by the end of the Void Recovery Phase that can lead to a further build up in axial stress.

6.2.2 Water uptake during Phase 1

The injected water volume data is shown in Figure 6.5. The symmetrical technological void was 2.5 mm all round the sample i.e. a 5 mm difference in diameter. This void space corresponds to 49 cm³ and is, therefore, filled by 49 ml of water during the initial flooding stage.

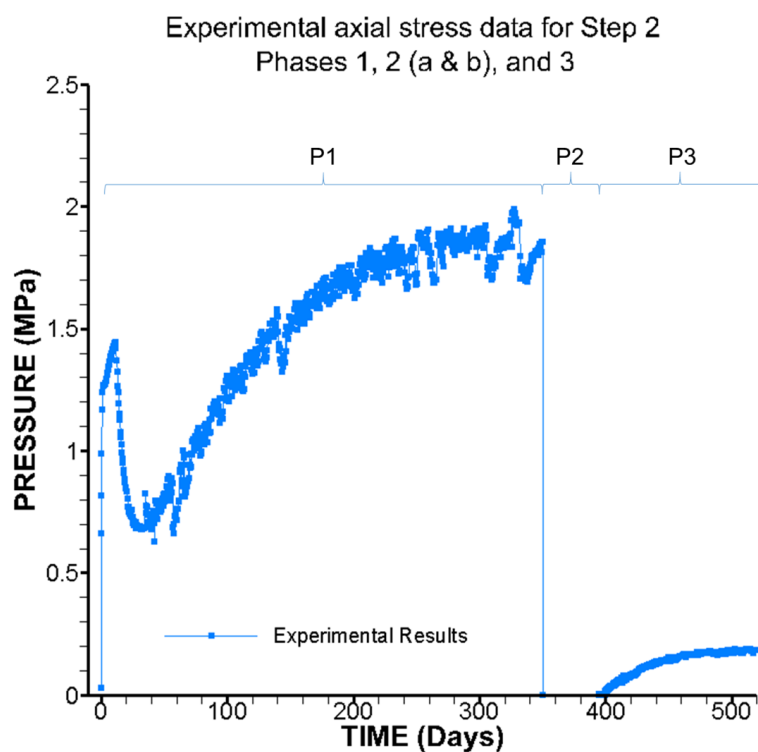


Figure 6.3: Axial stress data measured during the hydration phase of Step 2 mock-up test , after Wang [2012]. The data exhibit a reduction in axial stress from 12-30 days which has been interpreted as a wetting-induced plastic collapse phenomenon [Wang, 2012].

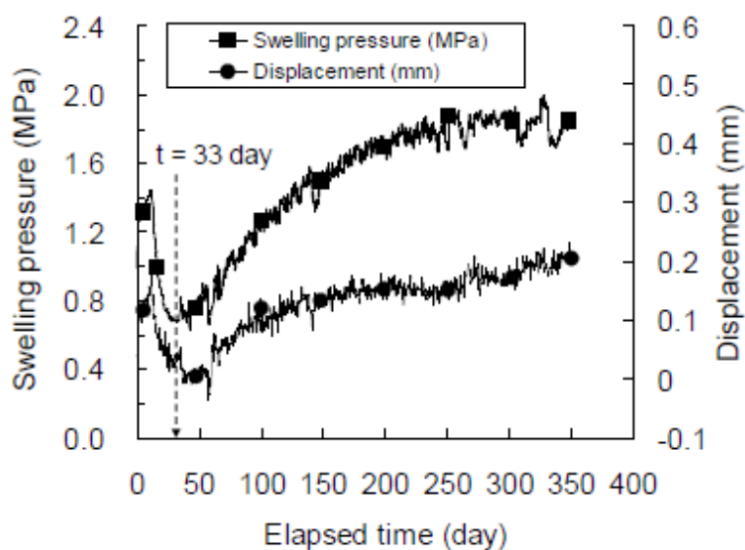


Figure 6.4: A graph showing the axial strain during the initial hydration phase of Step 2. The small measured strain in the Wang [2012] data is that of the Step 2 mock-up test and reflects the collapse process.

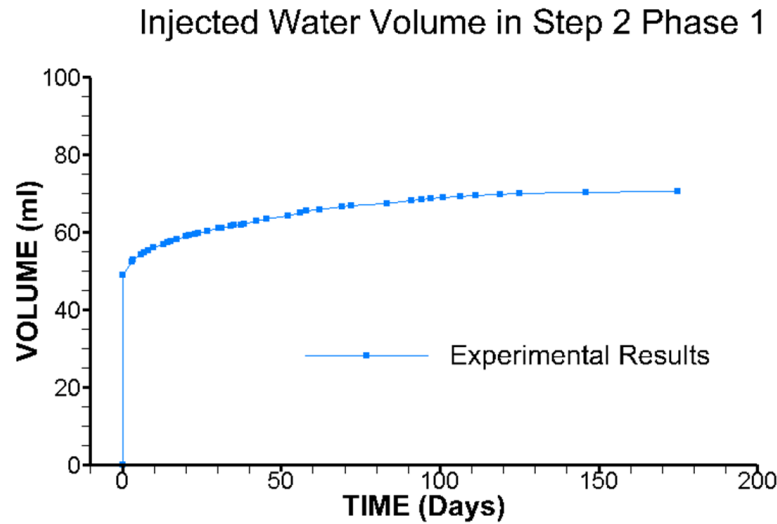


Figure 6.5: Measured injected water volume in the Step 2 mock-up test, after Wang [2012]. The technological void was initially flooded with 49 ml of water followed by further uptake of water by the bentonite.

Further hydration proceeds from the base of the sample and the subsequent uptake of water is into the bentonite. The rate of water uptake gradually reduces until no more water is taken up after *c.* 200 days [Wang, 2012], although this is not shown in the supplied data (Figure 6.5).

6.2.3 Axial displacement during Phase 2

Figure 6.6 shows the axial displacement measured during Phase 2a and Phase 2b. Upon unloading of the axial confinement an elastic rebound of < 2 mm is measured. This is followed by a gradual rate of axial strain as hydration proceeded from the base only. In order to accelerate the deformation, hydration was added from the top of the sample after 364 days [Wang, 2012]. The rate of axial deformation increased until the maximum 20% strain is reached after 395 days.

Axial displacement is driven by the expansion of the bentonite upon hydration. Consequently, at the end of Phase 1 the constant volume conditions result in an internal suction remaining within the sample that cannot be alleviated i.e. although the net suction has equilibrated to the boundary conditions resulting in no more water uptake or increase in swelling pressure, suction remains in the sample that is accessible once the confinement has been released during Phase 2a and 2b.

6.2.4 Expected key processes

The experimental results suggest the following key processes are active in this experiment:

- Stress build up with suction decrease / hydration.
- Rapid water uptake in the void before a more gradual infiltration.
- Reduction in axial stress with suction decrease i.e. wetting-induced collapse.

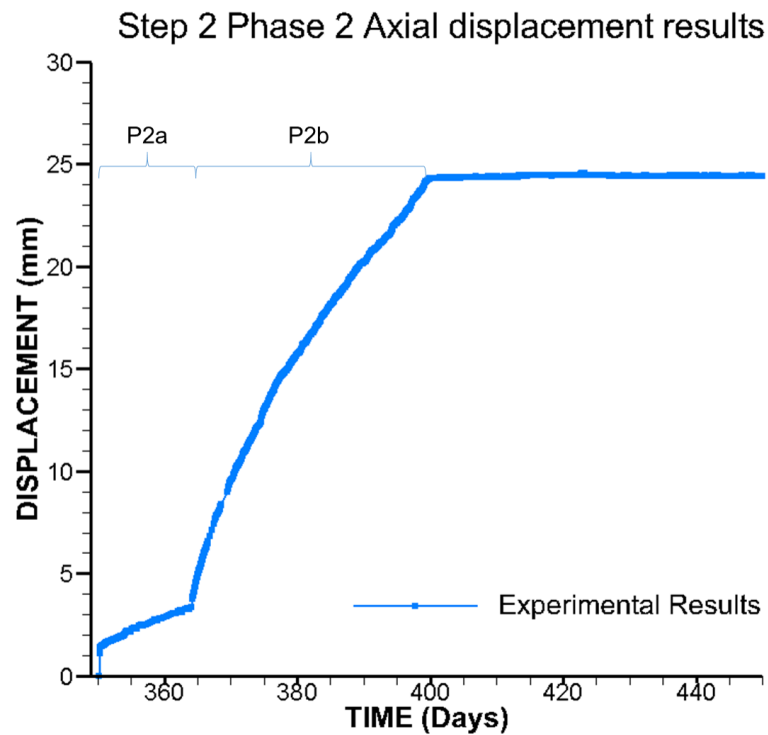


Figure 6.6: Measured axial displacement during Phase 2a and Phase 2b in the Step 2 mock-up test, after Wang [2012]. An initial elastic rebound < 2 mm is followed by a gradual axial expansion as the sample is hydrated from the base only. After 364 days, hydration from the top was introduced resulting in a greater rate of axial strain.

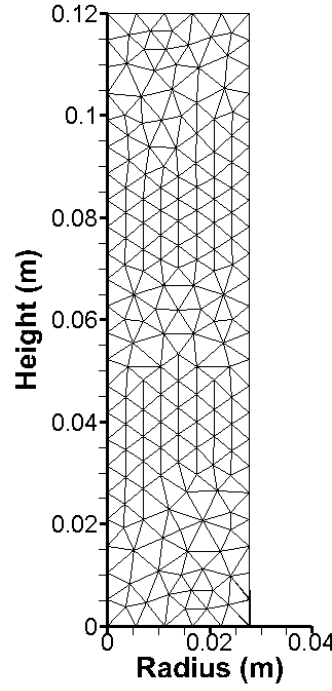


Figure 6.7: The 2D-axisymmetric mesh used to model the $1/10^{th}$ scale mock-up tests performed as part of the SEALEX experiments.

- Suction and elasticity driven deformation in the Void Recovery Phase.

The following sections present the method with which the experimental results are simulated.

6.3 Model set-up

A major feature of this experiment is the presence of the technological void, which must be considered in the model set-up. In this case, the symmetry of the void and the experimental set-up allows an axisymmetric representation of the system to be used. Therefore, a 2D-axisymmetric triangular mesh was generated using Gmsh [Geuzaine and Remacle, 2009], as shown in Figure 6.7. The axis of symmetry representing the centre of the sample is the left hand edge of the model. No specific representation of the void or the hydration cell were considered in the mesh of this experimental set up as specific boundary conditions were developed to represent these features.

6.3.1 Displacement dependent boundary conditions

One of the main considerations in modelling the Step 2 $1/10^{th}$ scale mock-up test and the Step 3 full-scale *in situ* experiment is the description of the technological void. There are a number possible methods to treat the void e.g. treating the void as a hydro-mechanical material that stiffens to the properties of steel as a function of strain, or as a stress boundary that increases in stress as a function of strain. However, the implementation of a Lagrangian moving mesh in this work allows the void to be described by a displacement dependent boundary condition

i.e. once a certain value of displacement that corresponds to the void space has been reached, the boundary becomes a zero displacement boundary.

A specific requirement for Step 2 is that this boundary is implemented for both hydraulic and mechanical processes. This is because the hydration from the technological void ceases once the technological void is filled with the expanding bentonite. The expansion of the bentonite is expected to be rapid (e.g. [Saba et al., 2014]) but not necessarily uniform for the whole length of the sample, especially as the base is also hydrated. Therefore, while the boundary conditions can be applied to the whole length of the pre-defined polyline at the start of the simulation, as the void becomes progressively closed the number of nodes that make up the polyline to which the boundary conditions are applied reduces. As a result the boundary condition function determines which nodes the pressure or displacement boundary condition is applied to.

For the axisymmetric model used for Step 2 the displacement of interest is in both the horizontal and vertical axes during Phase 1 and Phase 2 respectively. As such, the general boundary conditions can be described by the following expression:

$$BC_H = \begin{cases} s & \text{for } u < u_{max} \\ Q = 0 & \text{for } u \geq u_{max} \end{cases} \quad (6.1)$$

$$BC_M = \begin{cases} \sigma_c = 0 & \text{for } u < u_{max} \\ u = 0 & \text{for } u \geq u_{max} \end{cases} \quad (6.2)$$

where BC_H and BC_M are the hydraulic and mechanical boundary conditions respectively, s is the suction (Pa), Q is the flux (m^3/s), σ_c is the confining stress (Pa), u is the displacement (m), and u_{max} is the maximum displacement that corresponds to the size of the technological void i.e. the distance to the cell wall.

The displacement limit (u_{max}) is defined by the user along with the axis of displacement. The hydraulic boundary condition of suction is applied while the mechanical boundary condition allows volume change, but becomes a no-flow boundary when the zero displacement mechanical boundary condition is on. This means fluid can enter the radial boundary of the sample only when there is a technological void. Once this void is filled there is no hydraulic flow across this boundary.

As swelling is likely to be non-uniform with the base swelling more rapidly than the top, the boundary condition for both the hydraulic and mechanical processes is applied to the nodes that have not reached the maximum displacement limit. This limit is therefore used to include or exclude nodes from the polyline to which the boundary conditions are assigned. These boundary conditions are applied to the right hand boundary of the mesh during Phase 1 to represent the technological void, and also to the top surface during Phase 2a and Phase 2b to accommodate swelling up to 20% axial strain.

Describing the technological void in this manner results in the added requirement that the technological void must be filled by the expanding Lagrangian mesh at a rate that corresponds directly to the expanding bentonite in order to accurately model the water uptake from this void space. Too slow and the model takes up too much water, too fast and the model does not see enough water. The void is assumed to be filled with liquid water (as defined by the boundary conditions) and therefore does not account for the development of a colloid or gel

that has been observed experimentally [Saba, 2014].

6.3.2 Calculating injected water volume

The volume of injected water is determined from the flux through the boundary faces. The calculation of flux for an axisymmetric model is not currently implemented in OpenGeoSys (pers. comm. Wenqing Wang 2015). Fluxes calculated as if for a 2D plane strain model could be converted to an axisymmetric model by multiplication with the circumference of the cylinder if a constant mesh application was employed. However, this is not the case in this model, and additional complications are caused by the displacement dependent boundary conditions that shut off hydraulic flow once the technological void is filled. The current implementation does not take into account the changing number of nodes along the polyline and therefore would give an erroneous value of flux. The following calculation of the injected water volume is conducted as a post-processessing method.

Total injected water volume is the sum of the flux through the vertical boundary for the duration of the simulation in which the technological void is open, and the flux through the base boundary throughout the experiment. Flux is calculated from the velocity output of the model at each node along the polyline. The modulus of the velocity vector is calculated from the velocity output in each axis for each node (n):

$$|v|_n = \sqrt{(v_x^2 + v_y^2 + v_z^2)} \quad (6.3)$$

This is then converted to flux by multiplying by the area over which the flux has occurred. For the vertical polyline, this area corresponds to an integration distance (L) between nodes along the polyline (Figure 6.8) multiplied by the circumference of the sample at the integration point (node n):

$$Q_n = |v|_n L (2\pi r_n) \quad (6.4)$$

where r_n is the radius of the sample at node n , and (Q_n) is the flux (m^3/s) at node n . The integration distance (L) is calculated from:

$$L = \begin{cases} (y_{n+1} - y_n)/2 & \text{for end of polyline nodes} \\ ((y_{n+1} - y_n)/2) + ((y_n - y_{n-1})/2) & \text{for all other nodes on polyline} \end{cases} \quad (6.5)$$

where y is the y coordinate of the node n , and the subscripts n_{+1} and n_{-1} denote the nodes either side of node n .

As the flux is calculating the volume of water entering the sample, the flux along the vertical boundary only contributes to the injected water volume when the technological void is not filled. Hydraulic flow continues through the base for the duration of the experiment and is calculated for the axisymmetric assumption by determining the cross-sectional area through which flow occurs (Figure 6.8(b)). The total flux is the sum of the flux through each mini segment area shown as A .

Total injected water volume (V_w) is then calculated as a sum of the flux for each time step:

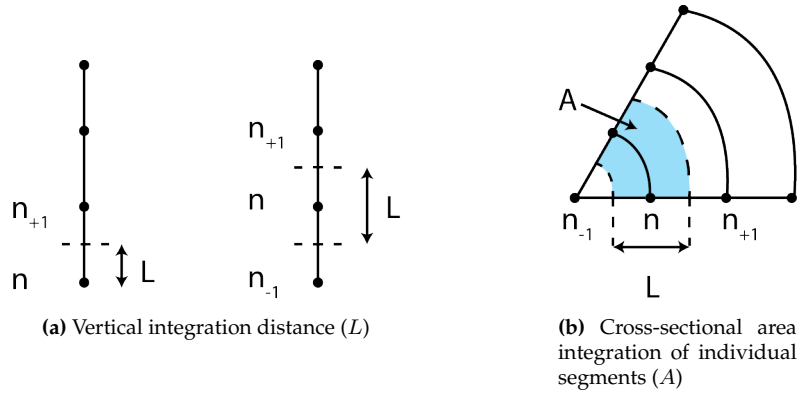


Figure 6.8: Schematic diagram of the calculation of the distance over which the flux is calculated in the vertical polyline (a) and the area through the base of the sample for the base polyline (b). The flux velocity vector is multiplied by the distance (L) and then by the circumference at the integration point in the vertical case, and multiplied by the calculated area in the base polyline case. The sum of the fluxes over each area gives the total flux

$$V_w = \sum_n^{\Delta t} \left(\frac{Q}{\Delta t} \right) \quad (6.6)$$

where n is the number of time-steps and Δt is the time-step length. Under constant volume conditions i.e. once the technological void is filled, the volume of water that can enter the sample is governed by the constant volume water retention curve. The Dueck suction concept calculates a water retention curve that takes into account the expansion of the sample to fill the technological void. However, the constant volume water retention curve as calculated in Step 1 indicates that the concept allows for the net suction pressure to change while no more water can be uptaken. As the velocity is calculated from the change in net suction, the injected water volume calculation is limited to the calculated volume within the sample when the model calculates 100% saturation.

6.3.3 Internal Strain Factor (Υ)

The HM model calibration presented for the Step 1 data is used to model the Step 2 mock-up test. However, the Step 1 mechanical model and coupling parameter (the internal strain factor Υ) were calibrated to consolidation tests performed on a bentonite-sand mixture with a dry density of 1.67 Mg/m^3 , and the Step1 mock-up test is performed at dry density of 1.97 Mg/m^3 . Numerous experimental investigations into the double structure of bentonite indicate that the volume of macro-pores at the higher dry density is significantly reduced in comparison to a lower dry density [Ferrari and Seiphouri, 2015, Lloret et al., 2003, Wang, 2012]. The internal strain factor is adjusted to reflect the difference in the crystalline swelling that can be accommodated by the reduced volume of macro-pores as hypothesised by Likos and Lu [2006]. At low water contents this results in a higher value of internal strain factor than calibrated in the Step 1 model as shown in Figure 6.9. The effect of the change to this function is to generate a larger confining stress under constant volume conditions. This is in-line with the observed increase in swelling pressure with increasing dry density [Komine and Ogata, 1996, Saba, 2014,

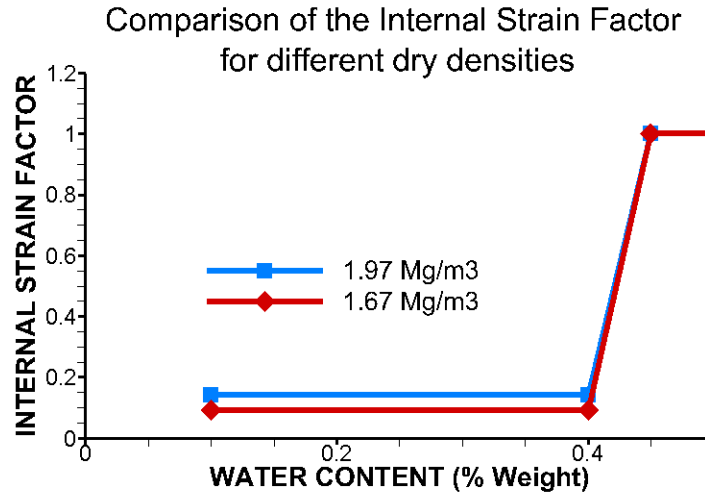


Figure 6.9: The water content dependency of the internal strain factor (γ) used in the coupled HM model for Step 2 compared to Step 1. The function reflects the difference in swelling processes with crystalline swelling dominant at water contents $<40\%$ and osmotic swelling dominant from $>40\%$ water content and varies with dry density due to the difference in macro-pore volume that can accommodate the crystalline swelling process.

Wang, 2012] (among many other authors). Furthermore, the increased confining stress results in less water being accommodated for a given value of suction, which is as one would logically expect [Wang, 2012].

6.3.4 Accounting for expansive collapse

The Step 2 axial stress results for Phase1 exhibit a wetting-induced collapse phenomenon that causes a reduction in axial stress as hydration proceeds. Figure 6.4 shows the close link between a reduction in axial stress and the axial strain evolution. This can be interpreted as a physical collapse process, or macro-structural compressive strains, responsible for the reduction in the axial stress [Lloret et al., 2003]. In order to represent these internal compressive strains within the confines of a macroscopic non-linear elastic model, a source term model is developed. A predictive method to activate the applied load is derived from a relationship between net axial stress and suction. Wang [2012] identified a linear relationship between the pre-consolidation pressure and net suction in the consolidation tests (Figure 6.10) which is given by:

$$\sigma_v = 0.1105(s) + 0.7455 \quad (6.7)$$

where σ_v is the net axial stress, and s is the suction.

The pre-consolidation pressure is considered to be the net axial stress at which yielding occurs, and can therefore be thought of as the onset of plastic deformation. In elasto-plastic models such as the Barcelona Basic Model (BBM) this relationship between suction and pre-consolidation pressure is used to define the Loading-Collapse curve and incorporates a dependency of the mechanical behaviour on hydration state [Alonso et al., 1990]. Applying this relationship as a Mohr-Coulomb type failure envelope provides a simple way to activate

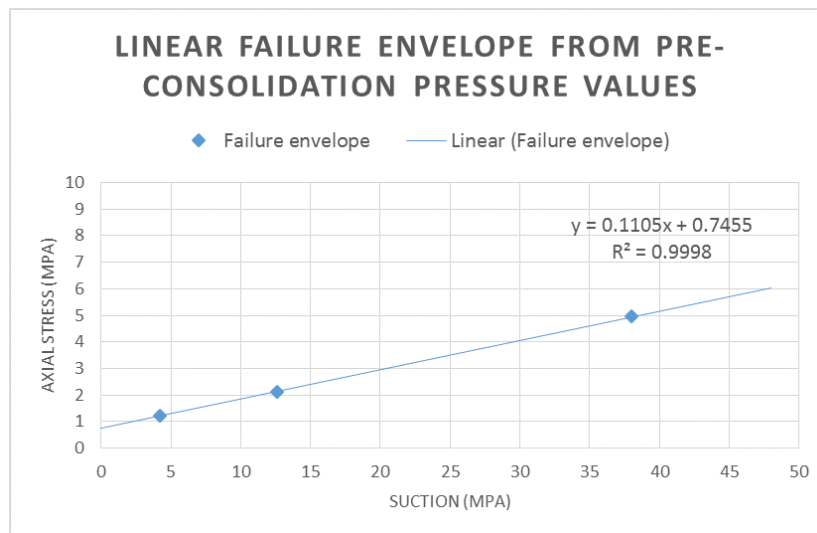


Figure 6.10: A linear relationship between suction and pre-consolidation pressure from the consolidation tests in the SEALEX laboratory tests after [Wang, 2012].

Table 6.1: An example of a curve used to calibrate the application of the source term to account for expansive collapse.

Percentage of sample > threshold	Applied source term (MPa)
0.00	0.00
30.00	0.00
50.00	0.30
70.00	0.45
100.00	0.45

or deactivate the source term to account for the wetting-induced collapse process. As this phenomenon occurs during hydration and the plastic behaviour in the consolidation tests is accounted for by the non-linear elastic model, the source term model is only activated during expansion. Every node in the mesh is evaluated for the axial stress-suction conditions and the source term applied as a function of the percentage of the sample that exceeds the threshold. An example curve is shown in Table 6.1 and represented graphically by Figure 6.11.

6.3.5 Parameterisation

The Step 1 hydraulic parameterisation is used throughout the Step 2 simulations and is shown in Table 6.2. The Step 1 hydraulic model was calibrated to an infiltration test on a bentonite-sand sample compacted to a dry density of 1.67 Mg/m^3 . The water retention curve calibration was also used, but the initial void ratio and coupling mechanism (the internal strain factor) are adjusted to take into account the change in void space associated with the higher dry density sample in Step 2.

The mechanical parameterisation is defined for both the non-linear elastic model and the non-linear elastic source term model in Table 6.3.

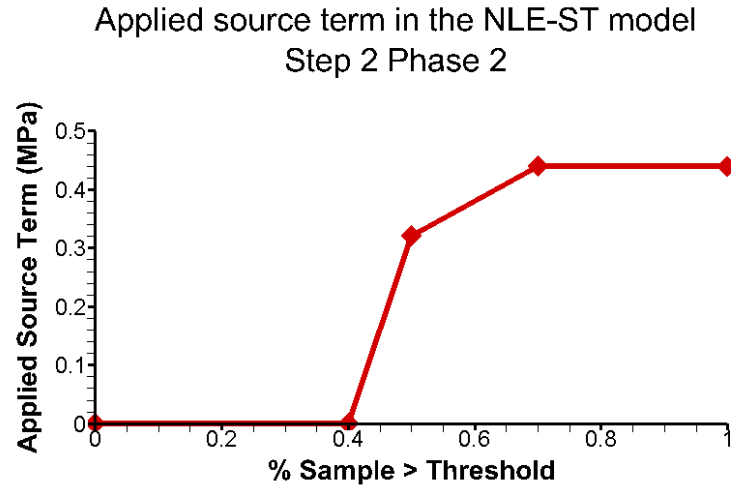


Figure 6.11: A graphical representation of Table 6.1 where a source term is applied depending on the % of the sample at a stress state that exceeds the failure envelope shown in Figure 6.10 and defined by Equation 6.7.

6.4 Results

The results for each phase of Step 2 are presented for both the non-linear elastic model and the non-linear elastic-source term model. Hereafter the non-linear elastic model will be termed the NLE model, and the model incorporating the source term for expansive collapse is termed the NLE-ST model.

Phase 1 is the initial hydration phase under constant axial volume and consists of the expansion of the sample into the radial technological void as hydration proceeds from both the void and the base of the sample. Once the void is filled hydration proceeds only from the sample base under constant volume conditions. Axial stress is measured by the piston at the top of the experimental cell over the whole diameter of the sample. The injected water volume is also measured over the duration of Phase 1. The model was deemed to be calibrated when the volume of injected water was well matched because during expansion the uptake of water is the driving mechanism in the coupled HM system.

Parameter	Value	Unit	Description	Origin
δ_p	1.2	nm	Ave. montmorillonite thickness	Liu et al. [2011]
C'_k	5.0	-	Pore shape factor	Liu et al. [2011]
ζ_p	$0.92M_b$	-	Montmorillonite fraction	Experimental data
m_a	5.5	-	Fitting parameter (Equation 3.38)	Calibrated
l	4.0	-	Fitting parameter (Equation 3.38)	Calibrated
η	3.8	-	Relative permeability power law	Calibrated

Table 6.2: The hydraulic parameterisation of the Liu et al. [2011] permeability function for Step 2. M_b is the mass fraction of bentonite in the bentonite-sand mixture as defined in the experiment [Wang, 2012].

Table 6.3: Mechanical parameters used to model Step 2. These parameters are those calibrated for a bentonite-sand mixture with a dry density of 1.67 Mg/m^3 . The initial void ratio and the parameter γ are varied to account for the density difference between Step 1 and Step 2 samples. σ_{th} is the stress threshold defined Equation 6.7.

Parameter Symbol	Value	Unit	Description	Origin
E_0	30.00	MPa	Initial Young's Modulus	Calibrated
ν	0.30	-	Poisson's Ratio	Calibrated
α_h	14.00	-	Hardening Parameter	Calibrated
α_s	3.50	-	Softening Parameter	Calibrated
d	3.00	-	Dimensionality factor	Calibrated
e_0	0.38	-	Initial Void Ratio	Experimental data
E_{min}	1.50	MPa	Minimum Young's Modulus	Calibrated
k_{red}	-1.00	-	Reduction factor	Calibrated
Υ	$f(M_w)$	-	Internal Strain Factor	Calibrated
σ_{th}	$f(\sigma_v, s)$	MPa	Stress threshold	Experimental data
ST	$f(\% > \sigma_{th})$	MPa	Source Term	Calibrated

6.4.1 NLE Model (no source term correction for plastic deformation)

The NLE model results for Phase 1 are presented in Figures 6.12 and 6.13. The axial stress develops immediately upon hydration but is over predicted by $c.2 \text{ MPa}$ as the model does not account for the expansive collapse process. The injected water volume is well matched for the initial stages of the hydration and the technological void is closed within 32 hours. However, further hydration in the model results in greater water injection than that observed in experiment. The elastic rebound calculated by the NLE model at the beginning of Phase 2a is much greater than in the experiment but the rate of subsequent deformation is similar to that observed (Figure 6.14). The NLE model calculates a sample at the end of Phase 1 that is mechanically weaker than the initial conditions due to the radial swelling. Combined with the over prediction of stored elastic energy, upon loss of confinement this results in too much rebound. The final strain of 20% is used as a displacement dependent boundary condition which leads the model to calculate the onset of Phase 3 after $c.385$ days. The subsequent stress build up follows a similar development to the experimental results although offset by 15 days (Figure 6.15). In order to compare the stress build up with the experimental results directly without the model predicted start of Phase 3, the axial stress results are temporally adjusted and presented in Figure 6.16. A good fit to the initial build up of stress is shown but the final axial stress calculated is under-estimated by 0.08 MPa - an error of nearly 50% .

During Phase 3 constant volume conditions are restored, and as such the build up of stress is due to the alleviation of suction. Therefore, the difference in the model calculation and the experimental results gives an indication of the difference in the calculated and actual suction pressure remaining in the sample after Phase 2.

6.4.2 NLE-ST Model (source term correction for plastic deformation)

The NLE-ST model results for axial stress development in Phase 1 are presented in Figure 6.17. Using the function in Table 6.1 the application of the source term accounts for a gradual

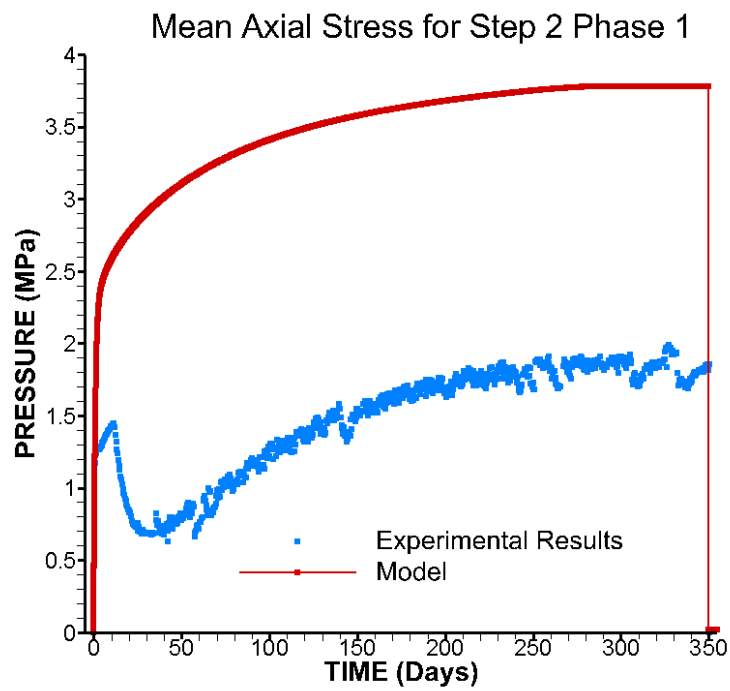


Figure 6.12: Modelled results for the build up of axial stress during Phase 1. The final stress is over-estimated by c.2 MPa

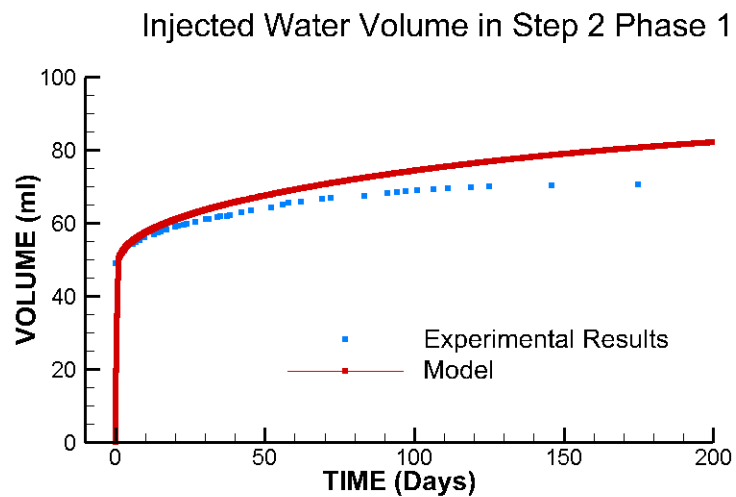


Figure 6.13: Modelled results for water uptake during Step 2 Phase 1. A good fit to the initial water uptake is achieved before model results progressively deviate from the experimental data.

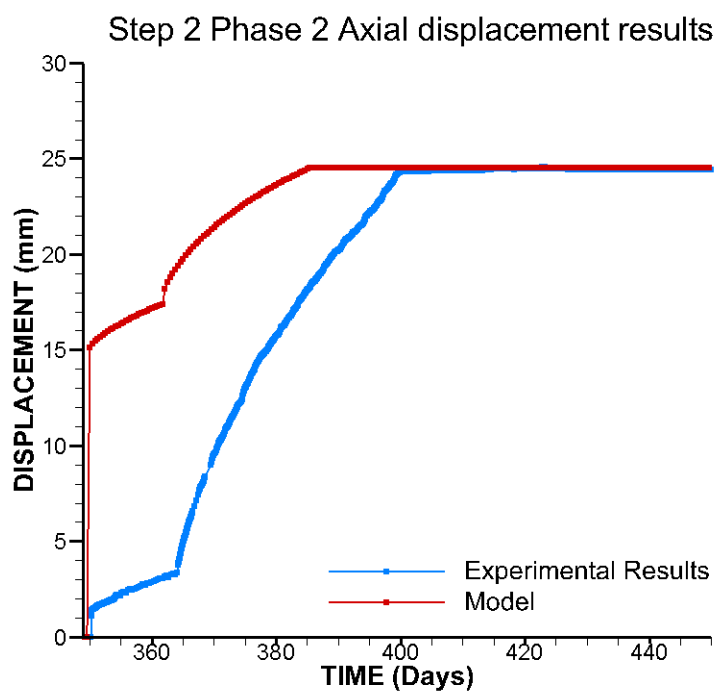


Figure 6.14: The vertical displacement calculated by the model over estimates the immediate elastic rebound but reproduces the gradients of further volumetric expansion and the increase in expansion rate at the start of Phase 2b.

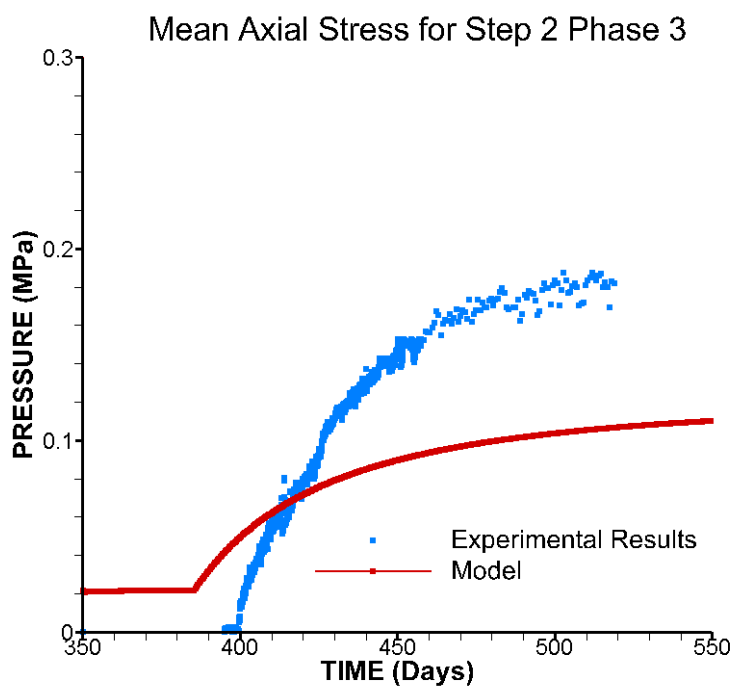


Figure 6.15: The axial stress build-up during Phase 3 starts too early as the 20% strain was reached before the experimental results due to the over prediction of the rebound in Phase 2a.

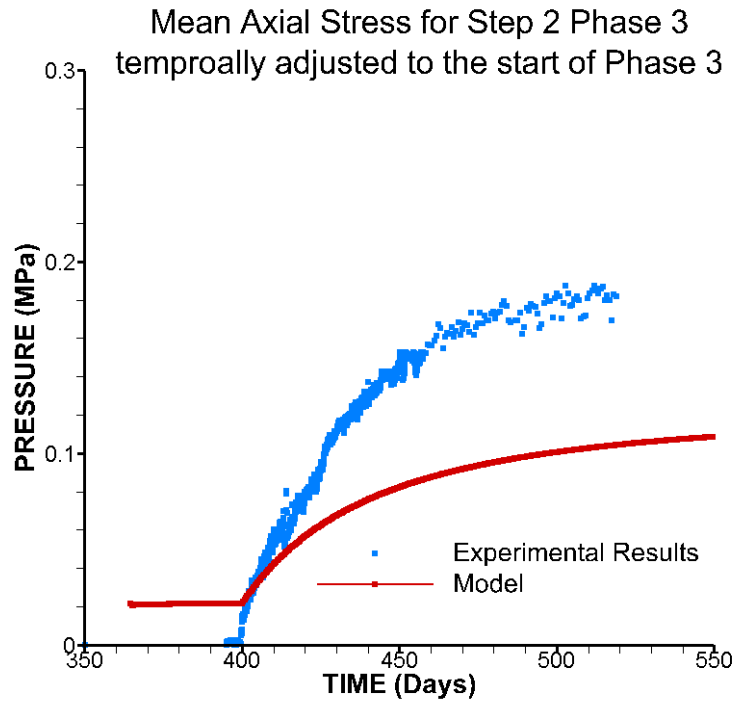


Figure 6.16: Temporally adjusted axial stress development in Step 2 Phase 3. The adjustment is made to compare the rate of axial stress development irrespective of the incorrect temporal calculation of displacement during Phase 2.

decrease in the axial stress after an initial peak of *c.* 2.3 MPa. This represents an over prediction of the initial peak stress but the onset of axial stress build-up and the final axial stress are well matched. The magnitude of axial stress loss is on the order of 0.9 MPa and develops over a similar timescale to the experiment. Axial stress begins to build up again once >70% of the sample exceeds the net stress- suction threshold defined by the pre-consolidation pressures of the consolidation tests. Interpreted in terms of the wetting-induced collapse phenomenon the axial stress reduces with compressive macro-structural strains but subsequently increases once the micro-structure expands to fill the voids. In this model the source term simulates this once the applied load becomes constant. The function used in this calibration defines this state to be after 70% of the sample exceeds the threshold i.e. there can be no more axial compressive strains with continuing alleviation of suction and this suction change therefore leads to a stress accumulation.

The injected water volume during Phase 1 is presented in Figure 6.18. The model calculates a good agreement to the experimental results although, in the same fashion as the NLE model, the water uptake is over-estimated towards the end of the experiment by *c.* 7 ml. The NLE-ST model provides a closer match to the experimental water volume injected due to the Dueck coupling procedure. The difference in the NLE and NLE-ST models in terms of water content is because the source term applies a compressive load to the base of the sample, which results in a lower permeability, and, through the Dueck suction coupling method results in a lower water content at the base of the sample.

The final gravimetric water content at saturation after the technological void was filled was calculated to be 23.0%. Wang [2012] state that the aim of the higher dry density of the

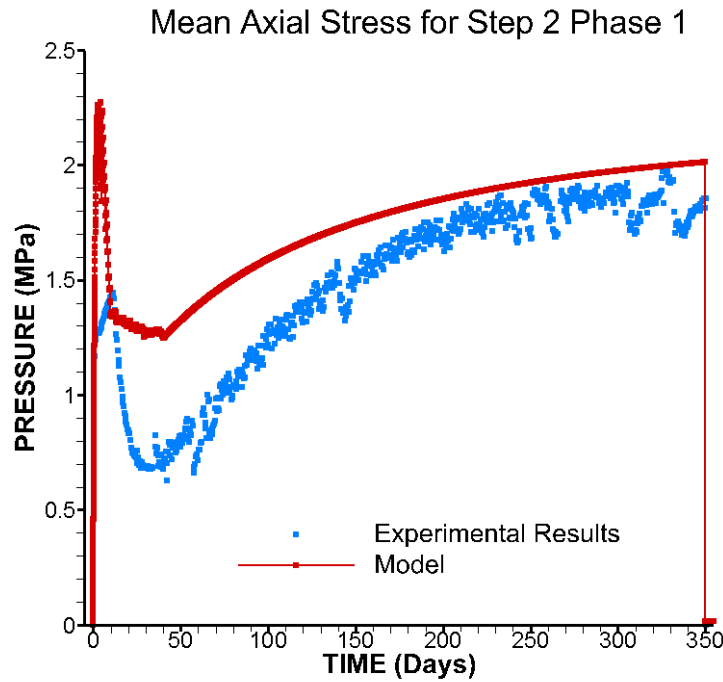


Figure 6.17: Modelled results for the build up of axial stress during Phase 1 with the NLE-ST model. The axial stress shows a gradual reduction before increasing until the final stress is well reproduced

initial sample was to reach an average dry density of 1.67 Mg/m^3 after the technological void is filled. The final gravimetric water content at saturation of a constant volume sample compacted to 1.67 Mg/m^3 was calculated in Step 1 to be 23.6%. The Step 2 results are within 0.6% gravimetric water content; an error of $<3\%$, which suggests the HM model is providing a good estimation of the stress influence on the hydraulic behaviour.

The elastic rebound during Phase 2a is again over-estimated by the NLE-ST model (Figure 6.19). Figure 6.19 also shows that the source term is progressively removed during Phase 2a as a result of the dependency of the application of the source term on the net axial stress-suction stress state. The removal of the axial confining stress leads to a change in net suction within the sample that moves the stress state below the stress threshold shown in Figure 6.10. This leads to more axial stress release and a further increase in net suction, which ultimately results in the majority of the sample below the stress threshold and the resulting deformation reaching the 20% strain value too quickly. As in the NLE model this leads to an accumulation of stress during Phase 3 that occurs too early in comparison to experimental results (Figure 6.20). The onset of Phase 3 occurs after $c.373$ days but results in a better fit to the development of axial stress in comparison to the NLE model. When the temporal inaccuracy of Phase 2 is adjusted for, the accumulation of axial stress during Phase 3 provides an excellent match to the experimental data (Figure 6.21).

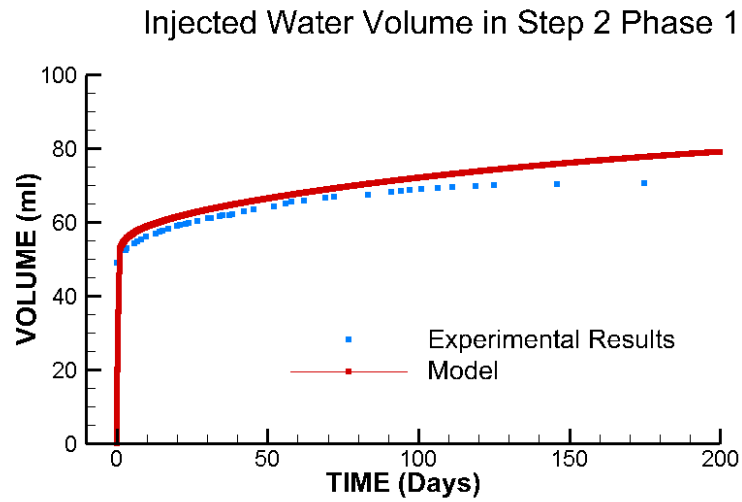


Figure 6.18: Modelled results for the injected water volume during Phase 1 with the NLE-ST model. The model calculates a good agreement to the experimental data although over predicts the water volume after 200 days (similar to the NLE model).

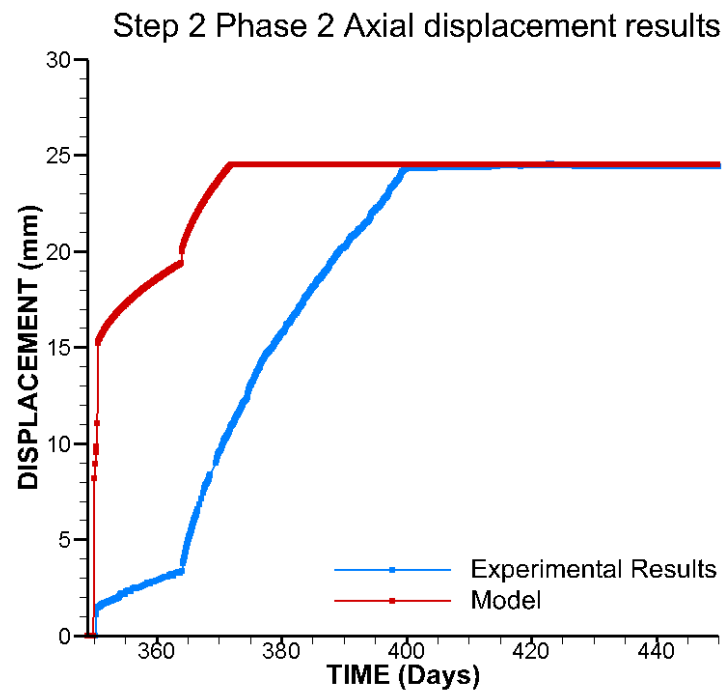


Figure 6.19: Modelled results for the vertical displacement during Phase 2. The model again overestimates the elastic rebound and calculates 20% strain significantly earlier than the experimental results.

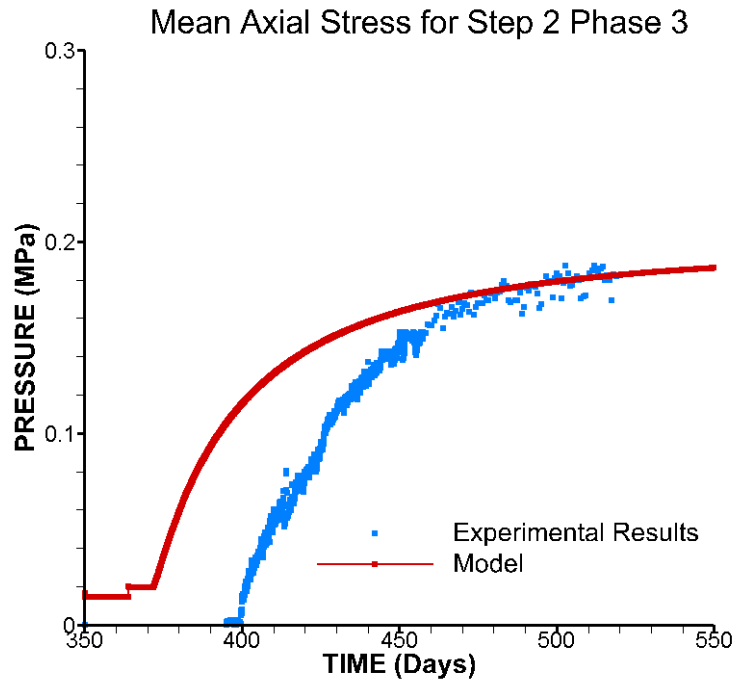


Figure 6.20: Modelled axial stress build up during Phase 3 of Step 2. The axial stress accumulation starts too early as the 20% strain was reached before the experimental results due to the over prediction of the rebound in Phase 2a.

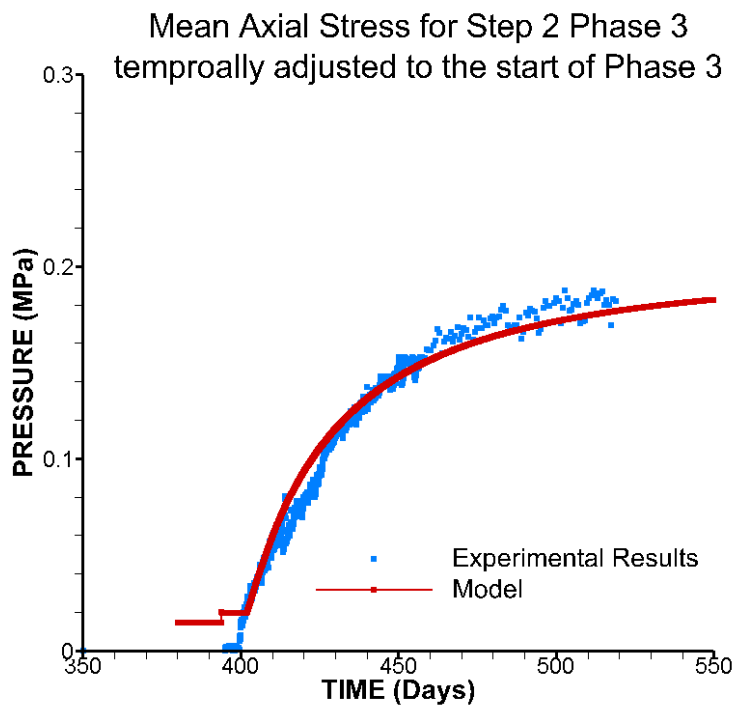


Figure 6.21: Temporally adjusted axial stress development in Step 2 Phase 3 calculated with the NLE-ST model. The adjustment is made to compare the rate of axial stress development irrespective of the incorrect temporal calculation of displacement during Phase 2.

6.5 Discussion

The hydro-mechanical conditions vary significantly during the different phases of Step 2. In Phase 1 radial free swell conditions with axial confinement dominate the behaviour and provide a challenge from a modelling perspective as no radial swelling/stress data were provided in the parameterisation step. Furthermore, this step included the transition from radial free swell conditions to radial confinement. During Phase 2 radial confinement persisted but this time free swell axial conditions prevailed, before Phase 3 returned to constant volume conditions. Nevertheless, using this simple model it is possible to draw some conclusions as to the main controls and driving forces during these changes in hydro-mechanical conditions. A summary of these is presented in Table 6.4.

The calculated gravimetric water content at the end of Phase 1 corresponds closely to the calculated gravimetric water content in the 1.67 Mg/m³ constant volume water retention test. Swelling into the technological void of a 1.97 Mg/m³ sample is designed to result in a final average dry density of 1.67 Mg/m³. The model calculates the water uptake as a function of the confining stress via the Dueck suction concept. The Dueck suction concept states a finite volume of water can be taken up as a function of the confining stress. The confining stress is a combination of both the mechanically applied load and the hydraulic stress from alleviated suction that is prevented from causing volume change. Under constant volume conditions the hydraulic stress is responsible for the build up of swelling pressure. The magnitude of this stress is governed by the internal strain factor (γ) which replaces the Biot coefficient in the solution (Chapter 4). A good agreement to the volume of injected water with both the

Phase	Process	Controlling factors
Initial Phase	Water Uptake	Bentonite permeability
	Axial stress evolution	Rate of expansion (filling of technological void) Development of confining stress Suction pressure within the sample Mechanical and Hydraulic stress states Failure curve dependent on both hydraulic and mechanical stress states for wetting-induced collapse
Void Recovery (1)	Elastic rebound	Stored strain energy, Mechanical stiffness of the material
Void Recovery (2)	Swelling	Mechanical stiffness of the material Bentonite permeability
Confinement	Axial stress evolution	Suction pressure remaining in the sample after Phase 2.

Table 6.4: Main controls on the hydro-mechanical behaviour in each phase of Step 2.

NLE and NLE-ST models and with the gravimetric water content corresponding to a 1.67 Mg/m^3 constant volume sample suggests that the variation of γ with dry density is a good representation of the change in hydro-mechanical behaviour between the two densities.

The axial stress during Phase 1 shows a build up of stress with a reduction in suction pressure within the sample. Both the NLE and NLE-ST models show this build up in stress to be a result of the hydro-mechanically coupled behaviour of a sample under axial confinement. However, the axial stress behaviour during Phase 1 also clearly indicates a wetting-induced collapse phenomenon that cannot be modelled with a non-linear elastic function. The application of a source term to account for the collapse behaviour allows a good fit to the axial stress results with the NLE-ST model. The main controlling factors in the parameterisation of the source term wetting-induced collapse behaviour are the definition of the failure curve, and the magnitude of the source term applied. The dependency of the failure curve on the stress state of the soil as a function of both the hydraulic and mechanical stresses enables the progressive reduction in axial stress to be recreated. This suggests that the temporal behaviour of the collapse is due to the evolution of the hydraulic and mechanical stress states and further emphasises the coupled nature to the physical behaviour as plastic mechanical deformation can be caused by the hydration process.

During Phase 2 the mechanical deformation is a function of both the stored elastic energy and the hydration state of the sample. In Phase 2a the experimental elastic rebound is small but both the NLE and NLE-ST models predict large rebounds due to the stored elastic energy remaining in the model at the end of Phase 1 and the reduction in stiffness of the material with the radial expansion to fill the technological void. The experimental results are similar to the non-linear behaviour observed in consolidation tests where there is an abrupt increase in mechanical stiffness upon unloading [Craig, 2004]. The theory of elasto-plasticity provides an explanation for this by separating the elastic and plastic processes such that plastic deformation does not influence the elastic properties of the sample. Consequently, when the loading is removed (in this case the axial confinement) the soil rebounds with the elastic properties before the onset of plasticity. Another factor in the calculation of the elastic rebound is the friction of the sample against the cell walls. However, the model set-up does not account for this and therefore translates all of the strain energy into deformation.

Finally, in Phase 3 the build up of stress is solely a function of the suction remaining within the sample. The model results show a consistent rate of stress accumulation during the initial onset of Phase 3 but only reproduces the final stress when the corresponding value of suction remains within the sample. Too little suction at the end of Phase 2 and not enough stress develops in Phase 3, whereas too much suction results in too large a stress build up.

6.5.1 Comparing the NLE-ST model to elasto-plasticity

The non-linear elastic source term model aims to account for the plastic behaviour occurring in the process of wetting-induced collapse. It is therefore worthwhile comparing this model to the elasto-plastic concept to note the similarities and key differences. In an elasto-plastic model one of two mechanical processes is occurring depending on the stress state of the soil. A three-dimensional failure surface is defined in terms of the net mean stress (p), deviatoric stress (q), and suction (s) [Alonso et al., 1990, 1999, Gens and Alonso, 1992]. This governs the elastic and plastic domains for loading, unloading, and expansive behaviours. At stress states

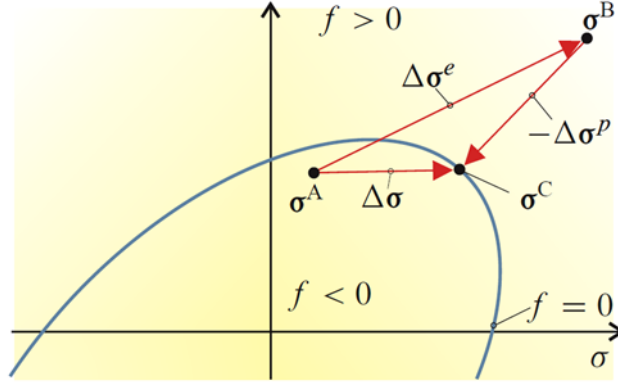


Figure 6.22: A diagram illustrating the concept of return mapping of stress in an elasto-plastic solution, after Clausen [2007]. The stress increment is calculated from the elastic stress and the plastic corrector stress to ensure that plastic deformation results in the stress state coinciding with the failure curve [Clausen, 2007].

within the failure surface elastic (or non-linear elastic) behaviour occurs and strain energy is stored. However, once the stress state of the sample breaches the failure surface, plastic deformation occurs [Alonso et al., 1990].

In an elasto-plastic model the total strain is a combination of the elastic and plastic strains:

$$\epsilon = \epsilon^e + \epsilon^p \quad (6.8)$$

where ϵ is strain, and the superscripts e and p refer to elastic and plastic processes respectively [Clausen, 2007].

This can be substituted into Hookes Law to give the elastic stress increment from the elasto-plastic strain as:

$$d\sigma = \mathbf{D}d\epsilon^e = \mathbf{D}(d\epsilon - d\epsilon^p) = \mathbf{D}d\epsilon - \mathbf{D}d\epsilon^p \quad (6.9)$$

where $d\sigma$ is the stress increment, $\mathbf{D}$ is the elastic constitutive matrix, $d\epsilon$ is the strain increment, and $d\epsilon^p$ is the plastic strain increment [Clausen, 2007].

Commonly, return mapping is used to determine the stress increment for a given time-step as a function of the failure criterion, the elastic strain and the plastic strain as shown in Figure 6.22. In this figure the stress increment is a function of both elastic and plastic components. The elastic stress increment corresponds to the stress increment that would be calculated if there was no failure criterion i.e. elastic behaviour to point σ^B , but if the stress state exceeds a failure criterion, the plastic stress increment (also known as the plastic corrector stress) returns the stress state back to the failure curve. The elasto-plastic method involves determining the plastic strains via a flow rule (defined in terms of a plastic potential and plastic multiplier) and a hardening law [Borja and Lee, 1990, Clausen, 2007]. The amount of strain that can be attributed to plastic deformation is then used to calculate a consistent elasto-plastic constitutive matrix which is used to calculate the stress state. The elasto-plastic constitutive matrix is essentially the equivalent material property that produces the same amount of calculated strain for the increase in elastic stress i.e. the contribution of plastic strain is removed from the calculation of the stress and stress is only calculated for the elastic deformation.

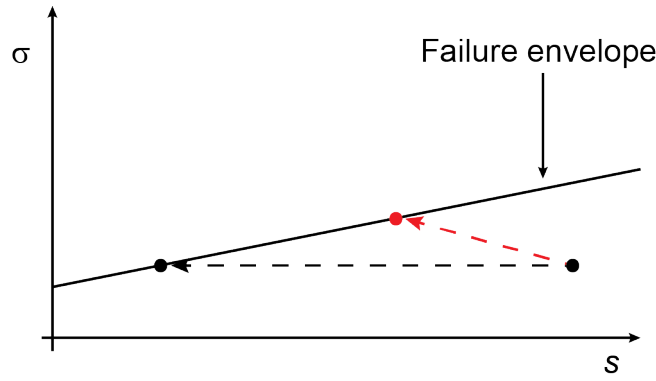


Figure 6.23: A graphical representation of the loading-collapse concept that is used to bring about expansive collapse in an elasto-plastic model and also the NLE-ST model developed in this work (σ is the stress (Pa), and s is the suction pressure (Pa)). The reduction in suction moves the stress state of the sample towards the failure envelope until it is breached. In this figure this is shown for a sample that does not develop swelling pressure (Black), and a sample that does develop a swelling pressure e.g. bentonite (Red).

In comparison, the NLE-ST model calculates the elastic stress directly from Hookes Law and accounts for wetting induced plastic collapse by applying a source term in the opposing direction to the axial stress development. This can be thought of as similar to the plastic corrector stress as it corrects the axial stress state to account for a collapse behaviour. Furthermore, the failure criteria used in the model for expansive collapse is similar to that of the loading-collapse curve in the elasto-plastic models. Expansive collapse is simulated in an elasto-plastic model because the failure envelope changes size with decreasing suction i.e. with increasing hydration [Alonso et al., 1990]. For example, the stress state of a sample may be situated in the elastic domain yet be brought to failure without a change in mechanical stress as the failure envelope reduces in size with increasing hydration (decreasing suction) [Alonso et al., 1990, Gens and Alonso, 1992, Wheeler and Sivakumar, 1995]. This is illustrated in Figure 6.23. The same definition of the suction dependence of the failure envelope during expansion is used in the NLE-ST model to account for wetting-induced collapse. Figure 6.23 shows an approximation of the failure envelope defined by the pre-consolidation pressures of the consolidation tests in the SEALEX experiments and the potential for wetting-induced collapse to be brought about by a reduction in suction. The red dashed line indicates the possible behaviour for a bentonite material under constant volume conditions where a swelling pressure develops upon hydration. As the suction decreases, swelling pressure increases and the stress state is moved towards the failure envelope. In the NLE-ST model these stress conditions are evaluated at each node and a source term approximating the plastic corrector stress is applied depending on the percentage of the sample that has exceeded these stress conditions.

However, the source term application for expansive collapse is different to an elasto-plastic model in a number of ways. Firstly, the elasto-plastic constitutive matrix is not calculated in the NLE-ST model which has the advantage of reducing the computational cost of this method but does not guarantee that the stress state is returned to a position on the failure envelope. Considering the source term to be similar in essence to a plastic corrector stress, it should be noted that this enters the equation system in a different location and therefore does not result in strain without stress. The equation for the increment of stress in terms of elastic and plastic

deformation after [Clausen, 2007] gives:

$$d\sigma = \mathbf{D}d\epsilon - \mathbf{D}d\epsilon^p \quad (6.10)$$

The stress relating to the term $\mathbf{D}d\epsilon^p$ is the plastic corrector stress and needs to be incorporated in the model in some way. If we then consider the finite element formulation rearranged to solve for the displacements, the difference between the elasto-plastic models and the NLE-ST model can be clearly seen:

$$\{\mathbf{u}\} = \underbrace{[\mathbf{K}]^{-1}}_{\text{EP alters this}} \times \underbrace{\{f\}}_{\text{NLE-ST alters this}} \quad (6.11)$$

In the elasto-plastic models the plastic strains are used to calculate an equivalent value of $[\mathbf{K}]^{-1}$ by return mapping, but in the NLE-ST model the change in stress caused by the application of a source term to account for wetting-induced plastic strain is incorporated into the force vector $\{f\}$.

The implication of this difference is two-fold. Firstly, the elastic material properties at the point of unloading in an elasto-plastic model are the same as at the onset of plasticity, but the NLE-ST model has material properties that relate to the total strain of the element i.e. including plastic strain. At the point of unloading this then results in a larger rebound than may be predicted by an elasto-plastic model. Secondly, the stored strain energy (stress) of the NLE-ST model includes the contribution from the plastic strain but an elasto-plastic model stores only the elastic strain energy. As a result, the NLE-ST model has more stored energy that can be released at the point of unloading than an elasto-plastic model, and therefore results in a large elastic rebound.

6.6 Conclusions

Overall, the NLE and NLE-ST models are able to capture the main features of the experimental behaviour for a variety of complicated hydro-mechanical conditions with the same parameter set as calibrated in conjunction with the Step 1 results. The moving mesh application is employed to define displacement dependent boundary conditions that model the swelling of the bentonite sample into the technological void. In order to model the expansive collapse phenomenon, a source term model with a failure criteria similar to that of the loading-collapse curve in elasto-plastic models is implemented. This failure criteria is defined by experimental results lending this method to future use in conjunction with laboratory consolidation tests. Furthermore, it is possible to identify the key processes occurring at each phase of the experiment and to ascertain the controlling factors that contribute to modelling the experimental behaviour. These are summarised in Table 6.4.

Chapter 7

Modelling Step 3 of the SEALEX experiments

This Chapter presents the modelling of a full scale *in situ* performance test using the non-linear elastic model developed in Chapter 4. Simulations provide a good agreement with experimental results for axial stress and relative humidity with a minor calibration to the permeability model. The non-symmetrical technological void in the experimental set-up is simulated with a 2D plane strain cross-section model that reproduces the non-symmetric distribution in relative humidity and suggests the development of heterogeneity within the sample as a result of differential swelling.

7.1 Introduction

The final modelling step of Task A of DECOVALEX-2015 involves the simulation of the full scale *in situ* performance test PT-A1. This was performed on the same bentonite-sand mixture used in the 1-10th scale mock-up test in Step 2. The core was made up of a number of compacted bentonite blocks with a diameter of 0.56 m and a total length of 1.20 m. A significant effort was made to ensure the core was as homogeneous as possible at the start of the test and the sample was heavily sensed to record data on relative humidity, and axial and radial stresses [Barnichon et al., 2012].

Figure 7.1 shows a schematic of the experimental design. The core was emplaced in a sub-horizontal drift with a diameter of 0.60 m. This resulted in a technological void around the specimen that, due to the horizontal geometry, was not symmetrical (as was the case in the mock-up tests) (Figure 7.2). The sample was held in place by a concrete plug sealed with an epoxy resin that prevented deformation along the axis of the excavated drift. Initially the experiment was flooded with a back pressure of 0.20 MPa to ensure the technological void was saturated, and subsequent hydration then proceeded through each filter stone at each end.

The location of the sensors is shown in Figure 7.2. Relative humidity sensors are distances of 0.22 m, 0.52 m, 0.82 m, and 1.12 m. Due to some experimental difficulties with some of the sensors, data was provided for the sensors at 0.22 m and 0.52 m. Axial stress was measured from a sensor located at the centre of sample ends at both 0.00 m and 1.20 m. In addition, radial stress was measured at three evenly spaced locations around the circumference of the

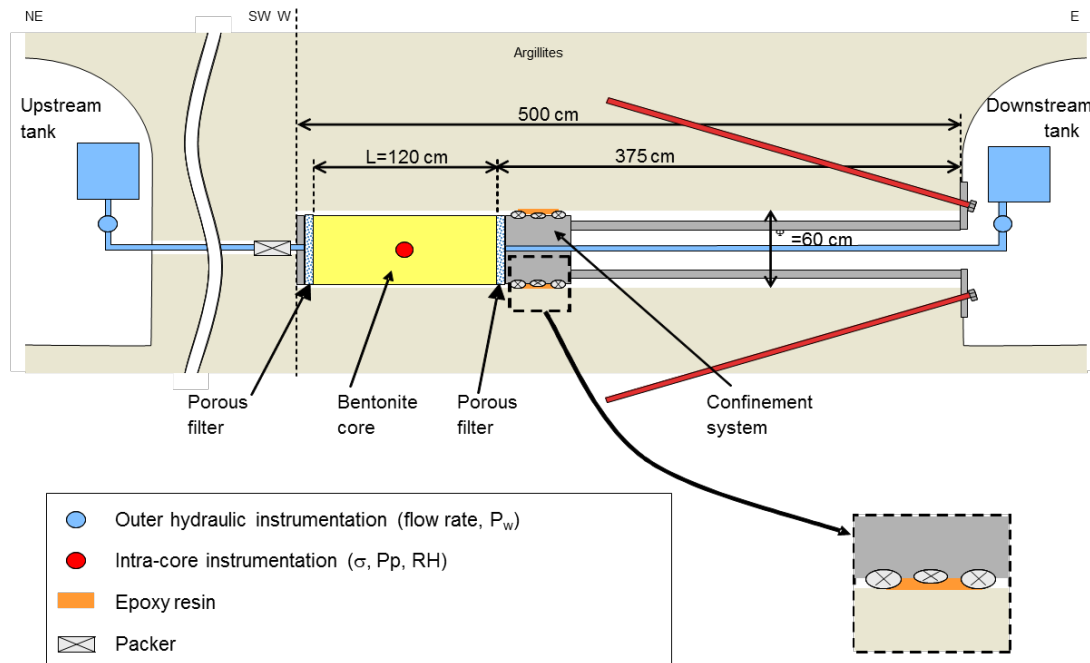


Figure 7.1: A schematic diagram of the PT-A1 performance test in the SEALEX experiments. The diagram shows upstream and downstream tanks, but in experimental reality these are the same tank. A concrete plug device prevents deformation along the axis of the borehole and filter stones allow hydration from the water tank. [Barnichon et al., 2012]

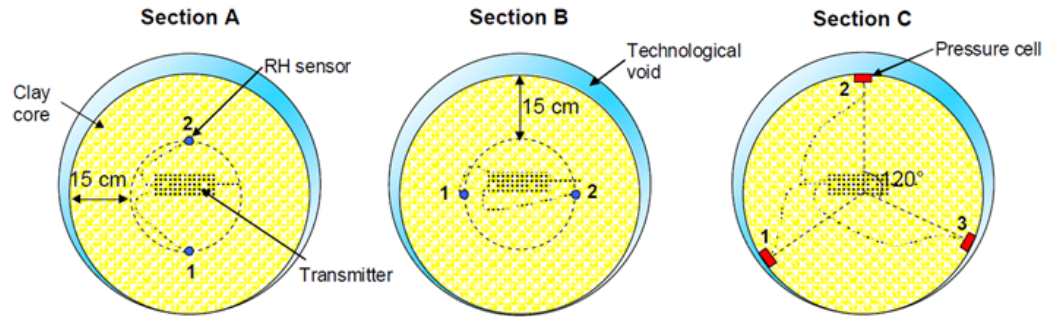
core at a length of 0.60 m as shown in Figure 7.2a-Section C.

7.2 Conceptual Interpretation of Experimental Results

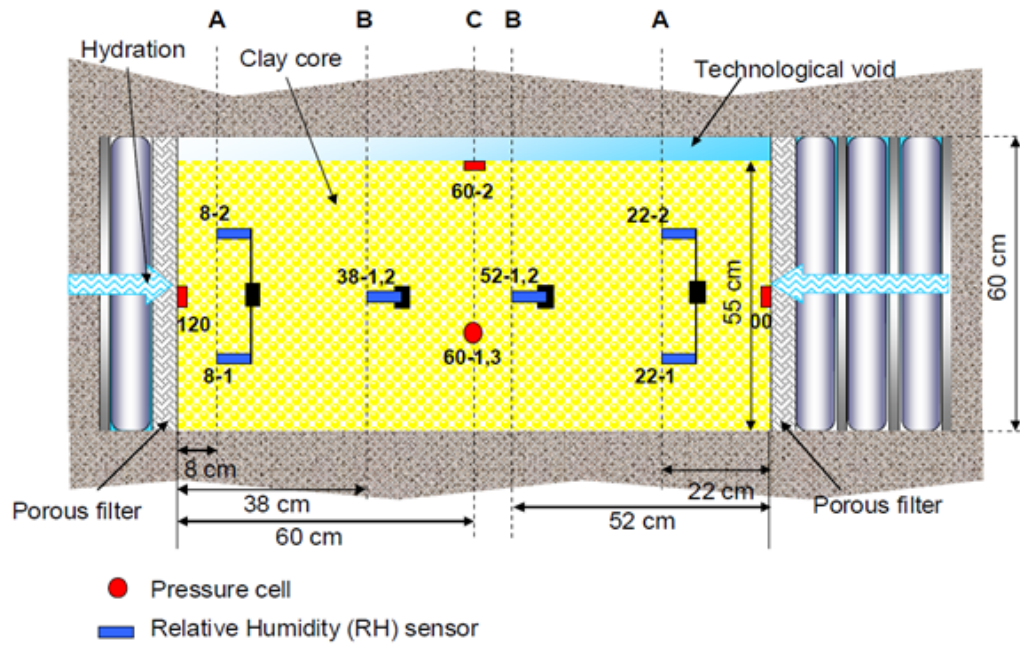
Experimental results are provided for the relative humidity at 0.22 m and 0.52 m along the sample (Figure 7.3), axial stress at each end, shown in Figure 7.4a, and radial stress at sensors around the centre of the sample, shown in Figure 7.4b.

7.2.1 Relative Humidity

The locations of the relative humidity sensors at 0.22 m along the sample leads to an expected dissymmetry as a result of the non-symmetrical technological void and subsequent differential hydration (Figure 7.2a Section A). Sensors 52-1 and 52-2 are located at the same height within the sample and were expected to have a similar hydration because the technological void size is similar each side (Figure 7.2a Section B). However, sensor 52-1 has a very different evolution to sensor 52-2. Due to the similarity of 52-2 to 22-1 and 22-2, it is possible that the evolution of sensor 52-1 is an experimental error that may be caused by a preferential pathway for hydration in the initial stages. For example, one interpretation is that a pathway along the contact between the blocks may have allowed the fluid to reach the sensor rapidly after *c.*25 days, leading to the jump in relative humidity. As the blocks expanded and filled the gap again, the suction gradient from the sensor to the surrounding bentonite may have become reversed so the fluid that initially reached the sample subsequently moved away from the sensor, leading to a reduction in relative humidity. However, as there are no data to corroborate possible



(a) Sensor location in cross-section at their respective positions along the length of the sample



(b) Sensor locations along sample length

Figure 7.2: Schematic diagrams of the instrumentation used in the PT-A1 performance test. Relative humidity sensors are located at different radial distances (a) and along the length of the sample (b). Axial stress sensors are located in the centre of each end and radial stress sensors located equally spaced around the circumference of the sample at Section C (a) [Barnichon et al., 2012, Saba, 2014]

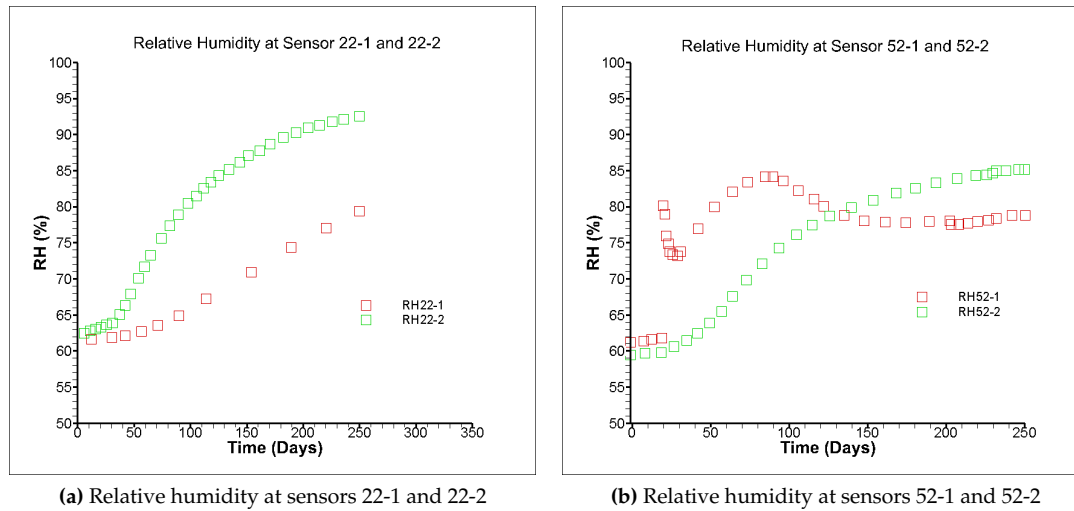


Figure 7.3: Experimental results for relative humidity at sensors 22-1 and 22-2 (a) and sensors 52-1 and 52-2 (b) measured during the PT-A1 performance test.

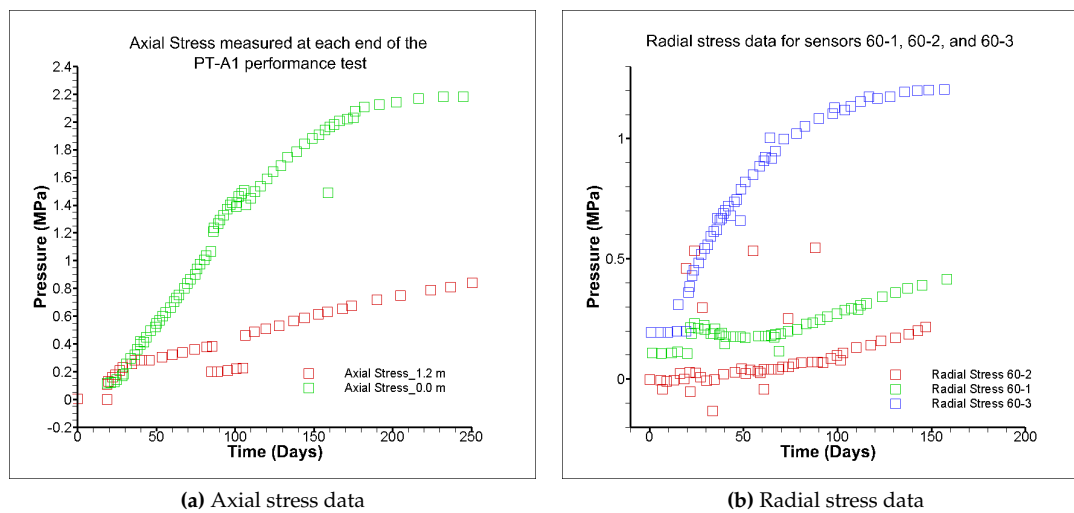


Figure 7.4: Experimental results for axial stress (a) and radial stress (b) as measured in the locations shown in Figure 7.2 during the PT-A1 experiment.

hypotheses, the data for RH22-1, RH22-2, and RH52-2 are used to compare to model results.

7.2.2 Axial Stress

Axial stress is calculated for both ends of the sample; at 0.00 m and at 1.20 m. Wang [2012] reported that the experimental hydration was stopped after the initial flooding of the technological void as a lateral packer was not fully inflated. The infiltration from each end began after 20 days. Accordingly, the experimental results indicate a time lag of axial stress build up of 20 days (Figure 7.11). The axial stress data also show a non-symmetric evolution, with stress development at sensor 0.0 m following a similar pattern to that of the sensor at 1.2 m until *c.*35 days, after which, they diverge. Axial stress at 0.0 m then develops at a greater rate than as recorded at the sensor at 1.2 m, leading to a pronounced, and as yet unexplained, dissymmetry between each end (Figure 7.11). The experimental conditions are designed to be symmetrical at each end with respect to the hydration and axial confinement. However, the results indicate a significant difference between the two final axial stress values. It is not known why this behaviour is recorded, and it is also hard to interpret. For example, possible explanations include the development of friction of the core along the base of the excavated drift during volume change, the potential extrusion of bentonite from one end into uncharacterised/unknown additional voids, or the heterogeneity of the bentonite core. There is also a degree of experimental scatter between 85 and 105 days where the two stress sensors calculate an opposite behaviour. Neither stress sensor shows the same collapse behaviour as seen in Step 2 in the small scale mock-up test, and due to the difficulty in interpreting the results, it is difficult to discern whether the model should try to predict the results for the sensor at 1.2 m, or at 0.0 m, or both. The unknowns in the interpretation of the data could result in a potential source of error in the modelling.

7.2.3 Radial Stress

The radial stress is that which acts directly outwards from the centre of the sample. The experimental data are shown in Figure 7.4b for each sensor 60-1, 60-2, and 60-3 (location shown in Figure 7.2a Section C). Sensors 60-1 and 60-3 were theoretically located at the same height in the sample, and with the same diameter technological void. Consequently, they were expected to give similar radial stress results. However, there is a clear difference between the measured stress at each sensor in both the final stress and also the initial stress conditions. This could be due to a rotation of the core during emplacement that caused the sample to be non-symmetrically arranged. Once again, the unknowns in the data could be a potential source of error for the application of a numerical model

The experimental data indicate that the technological void is filled at sensors 60-1 and 60-3 after *c.*20 days. Calculating the location of the sensor using the method of describing the boundary conditions (in the following section) in Equation 7.2 and comparing this to the location of the radial boundary reveals that the distance to the boundary at sensors 60-1 and 60-3 is 0.01 m. This is a quarter of the 0.04 m distance to the boundary for sensor 60-2 but the radial stress begins to build up at sensor 60-2 after just 50 days. Extrapolating a linear rate of expansion from the void closure over the shortest distance would suggest the void would become closed at sensor 60-2 after 80 days. As the measured closure is significantly shorter, and the development of radial stress at sensor 60-2 also shows a very gradual rise (as opposed

to the steep jump observed for sensor 60-3) this may be a representation of the development of a bentonite gel in the void space. The gel may act as a weak mechanical material that expands at a greater rate, until further expansion causes gradual compaction e.g. as observed in small scale experiments [Saba, 2014].

7.2.4 Expected key processes

The experimental results exhibit a number of behaviours that are difficult to interpret with much confidence. As a result, the key processes identified are restricted to the fundamental interpretation of the driving forces in the system:

- Stress development with suction decrease / hydration.
- Differential water uptake dependent on the size of the void space.

In addition, the results suggest a possible development of a bentonite gel, and a non-linear expansion rate in the technological void. The following sections present the method with which the experimental results are simulated.

7.3 Model set-up

The non-uniform technological void represents a specific challenge for the modelling of Step 3 as the axisymmetric model developed for Step 2 is not able to reproduce the geometry of the technological void. In order to gain an understanding of the effect of the non-uniform technological void without extending the model to three-dimensions, a two-dimensional slice at 0.60 m along the core is also modelled. Figure 7.5 shows the 2D axisymmetric mesh and the 2D cross-section mesh generated in Gmsh [Geuzaine and Remacle, 2009]. The axisymmetric mesh has a radius of 0.28 m and, as such, makes the assumption of a uniform technological void. Although the experiment was conducted in a sub-horizontal drift, the mesh is vertically oriented to make use of the axisymmetric calculations in OpenGeoSys. However, hydraulic flow has been shown to be independent of gravity in the hydration of bentonites as the main driving force is the internal suction pressure generated by the physico-chemical properties of the montmorillonite clay. The 2D plane strain cross-section model has a diameter of 0.56 m to reflect the radial geometry of the compacted bentonite core.

7.3.1 Displacement dependent boundary conditions

The same boundary conditions used in the modelling of Step 2 have been used in the axisymmetric model for Step 3. Hydraulic boundary conditions are applied to the base and top of the model to account for liquid water, and the displacement dependent boundary condition is applied to the right hand axial boundary. Zero displacement boundaries are applied to the top and base of the sample and activated along the right hand axial boundary once the technological void has been filled. The 2D slice cross-section model has only one boundary which can be described by the displacement dependent boundary conditions. In the axisymmetric models the displacement limit was dependent on displacement in a single direction but the radial swelling in the 2D cross-section requires a different description of the displacement limit. A

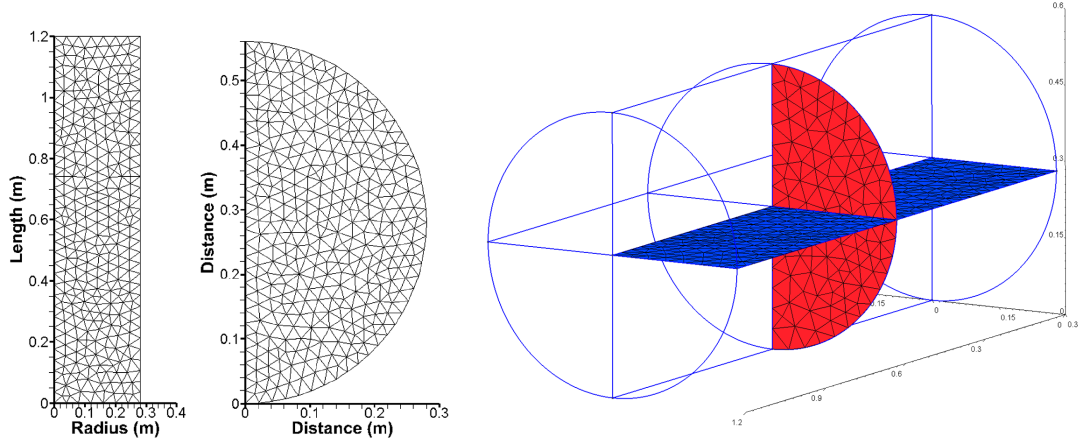


Figure 7.5: Finite element meshes generated for the modelling of the SEALEX experiment PT-A1. An axisymmetric mesh (left) and 2D slice cross-section mesh (centre) are generated because the experiment requires a description of the non-uniform technological void. The location of the meshes with respect to the 3D core is shown (right)

radial swelling limit is defined based on the circumference of the excavated drift hole, which is defined by the equation of a circle:

$$r^2 = (x - h)^2 + (y - k)^2 \quad (7.1)$$

where r is the radius of the circle, x and y are the locations of points in the cartesian co-ordinate system, and h and k are the cartesian coordinates of the centre of the circle. This is shown graphically in Figure 7.6. The circumference of this circle then becomes the limit of the nodal locations i.e. a node is not able to be displaced to a location outwith this circumference. In implementing this boundary condition the assumption is made that the drift hole is perfectly circular, which is a necessary simplification as there are no data regarding the shape of the excavated drift. However, the shape of the expanding bentonite is not restricted until the boundary is reached. This, therefore, allows for the dissymmetry of the technological void in the model set up.

The sample is assumed to be symmetrical in the vertical axis of the cross-section shown in Figure 7.5. Making use of the symmetry of the circle to reduce the mesh to a semi-circle, and assuming that the centre of the circle is around the axis $x = h = 0$ and the circumference passes through the origin, Equation 7.1 is rearranged to give the value of x for any value of y :

$$x = \sqrt{r^2 - (y - r)^2} \quad (7.2)$$

The x coordinate of the boundary node is then compared to the calculated x location determined from the y coordinate of the boundary node. If the x value exceeds or equals the circumference at that value of y then the boundary conditions become active/non-active (depending on the process).

Specific consideration is required for the nodes located along the central axis of the 2D slice cross-section i.e. the ends of the polyline defining the radial boundary. As these nodes are also connected to the central axis of rotational symmetry of the model, deformation can only occur in the y directions. Consequently the boundary condition for these nodes requires definition

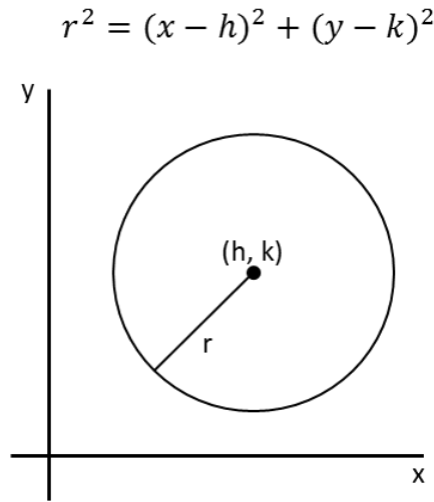


Figure 7.6: A graphical representation of the equation of a circle that is used to define the circumference of the excavated drift in Step 3 modelling.

with respect to the y coordinate location. The circumferential value of the y coordinate for an x coordinate of 0.0 is calculated from;

$$y = \left(\sqrt{r^2 - (x - h)^2} \right) + k \quad (7.3)$$

for a node location above the centre of the circle, and;

$$y = -1 \left(\left(\sqrt{r^2 - (x - h)^2} \right) + k \right) \quad (7.4)$$

for a node location below the centre of the circle. For the node above the centre of the circle the switch for the boundary condition occurs when the model y coordinate is equal to (or greater than) the circumferential y coordinate i.e. allowing upwards deformation, but the switch for the node below the centre of the circle is triggered when the model y coordinate is equal (or less than) the circumferential y coordinate i.e. downwards deformation. In practice the location of the node at the base of the circle is in contact with the drift wall and as such the hydraulic boundary is off and the mechanical boundary is on from the start.

7.3.2 Parameterisation

The hydraulic model described in Step 2 modelling is again used to simulate the up-scaled Step 3 experiment. The free swell water retention properties calibrated in Step 1 are combined with the Liu et al. [2011] permeability model to determine the axial stress at each end of the sample, the relative humidity at sensors 22-1, and 52, as well as the radial stress at sensor 60-3 (axisymmetric model) and sensor 60-1 (2D plane strain slice cross-section model). Once again, calibration was performed to the hydraulic process as this is driving the expansion into the technological void and the corresponding build up of stress when partially and fully confined. The hydraulic model was adjusted to match the relative humidity profiles at both sensor 22-1 and 52 by an edit to the permeability model. The parameterisation is shown in Table 7.1 with the Step1 permeability model values in brackets for comparison. The calibration parameter m_a is reduced, which results in an increase in calculated intrinsic permeability.

Parameter	Value	Unit	Description	Origin
δ_p	1.2 (1.2)	nm	Ave. montmorillonite thickness	Liu et al. [2011]
C_k	5.0 (5.0)	-	Pore shape factor	Liu et al. [2011]
ζ_p	0.92 M_b (0.92 M_b)	-	Montmorillonite fraction	Experimental data
m_a	5.0 (5.5)	-	Fitting parameter (Equation 3.38)	Calibrated
l	4.0 (4.0)	-	Fitting parameter (Equation 3.38)	Calibrated
η	3.8 (3.8)	-	Relative permeability power law	Calibrated

Table 7.1: The hydraulic parameterisation of the Liu et al. [2011] permeability function for simulation of Step 3. M_b is the mass fraction of bentonite in the bentonite-sand mixture as defined in the experiment [Wang, 2012]. The Step1 parameters are included in brackets for comparison to show the minor change in permeability required to fit the relative humidity data.

Table 7.2: Mechanical parameters calibrated to the consolidation tests for Step 1 and used in both Step 2 and Step 3. The Internal Strain Factor parameterisation is the same function of water content for this modelling step as used in Step 2.

Parameter Symbol	Value	Unit	Description	Origin
E_0	30.00	MPa	Initial Young's Modulus	Calibrated
ν	0.30	-	Poisson's Ratio	Calibrated
α_h	14.00	-	Hardening Parameter	Calibrated
α_s	3.50	-	Softening Parameter	Calibrated
d	3.00	-	Dimensionality factor	Calibrated
e_0	0.38	-	Initial Void Ratio	Experimental data
E_{min}	1.50	MPa	Minimum Young's Modulus	Calibrated
k_{red}	-1.00	-	Reduction factor	Calibrated
Υ	$f(wc)$	-	Internal Strain Factor	Calibrated

Axial stress data for sensor 0.0 m shows an elastic behaviour without evidence for plastic collapse. As a result, the non-linear elastic model, without considering the source term to account for plastic collapse, was used to model the mechanical behaviour of Step 3. The parameter set used is the same as that calibrated to the Step 2 experiment and is shown in Table 7.2. The coupling parameter, internal strain factor (γ), is the same function of water content as used in Step 2 for the 1.97 Mg/m³ dry density sample and shown in Figure 6.9 (Chapter 6).

7.4 Results

The results of the NLE model are presented for relative humidity, axial stress, and radial stress for both the 2D axisymmetric model and the 2D plane strain slice cross-section model. As in Step 2 the model is calibrated to the hydraulic process, in this case, the relative humidity, but no change is made to the mechanical parameterisation.

7.4.1 Relative humidity

Results for Step 3 include both the axisymmetric model and the 2D plane strain slice cross-section model in order to investigate the effect of the technological void on the hydro-mechanical behaviour. The 2D-slice model simulates a slice at 0.6 m length along the core and does not include the hydration from the base of the model. Therefore, the calibration is performed to

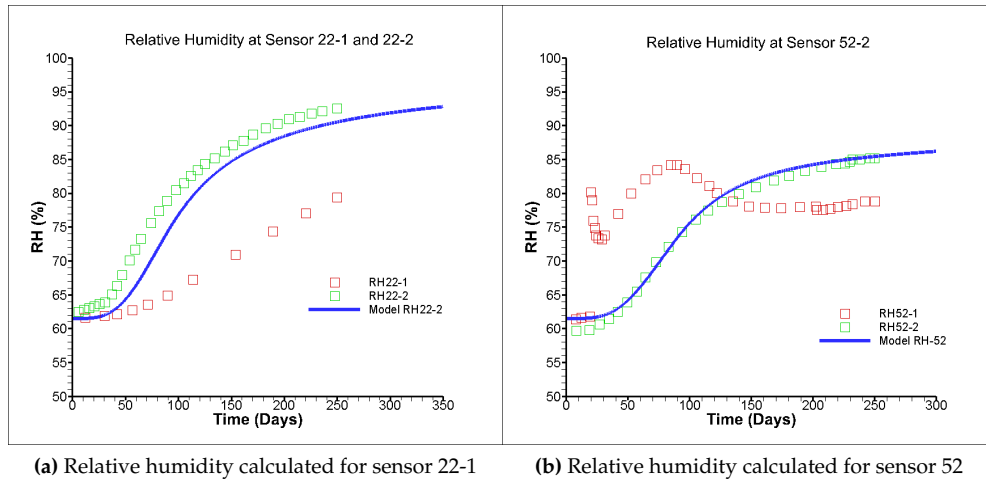


Figure 7.7: Model results for relative humidity at sensors 22-1 (a) and 52 (b). The model calculates a good fit to the data with the gradient of relative humidity increase and final relative humidity values well matched. The minor discrepancies between the results and the data are caused by the different starting relative humidities measured in the experiment and the uniform initial conditions value in the model.

the relative humidity data at RH52-2 because this is closest to the location of the 2D slice cross-section and least affected by the end hydration. The relative humidity results calculated for sensors 22-1 and 52 in the axisymmetric model represent an averaged value based on the uniform technological void. These are compared to experimental data in Figure 7.7. The model calculates a good fit to the experimental results for sensors at both 22-1 and 52 with the elevated permeability model. The rate of relative humidity increase is well matched with just a slight offset in model and experimental values due to the different initial relative humidity values and a short time lag in the model results. Final values of relative humidity are well matched using a model in which the hydraulic boundary condition is removed when the technological void becomes filled. This suggests that there is very little hydraulic contribution from the host rock.

The axisymmetric model is not able to capture the non-symmetric nature of the relative humidity data for sensors 22-1 and 22-2. This is, again, due to the geometry of the model set up which does not consider the non-symmetric technological void. In the experiment, sensor 22-2 is situated in the bottom half of the sample where there is less water available for hydration because the technological void is smaller. The location of the sensors is shown in Figure 7.8 which portrays the 2D slice cross-section mesh used in the modelling. Using the moving finite element mesh application, these data points move with the calculated deformation as one might expect the sensors in the sample to move with the deforming sample. If the rock has little or no hydraulic contribution the relative humidity increases at a slower rate for sensor 22-1.

In contrast to the axisymmetric model, the 2D slice cross-section model is able to simulate this difference in relative humidity caused by the non-symmetric technological void as the geometry of the void is explicitly modelled with the displacement dependent boundary conditions (Figure 7.9). The calculated relative humidity at sensor 52-2 in the 2D slice cross-section is also shown in Figure 7.9(b). The results recreate the magnitude of the dissymmetry

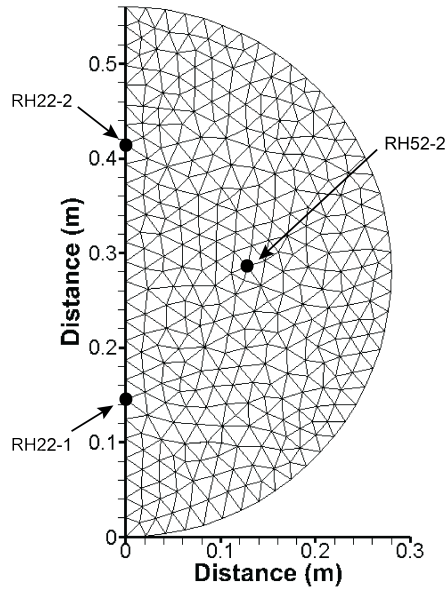


Figure 7.8: The 2D slice cross-section finite element mesh used to model the non-symmetric technological void in Step 3. The location of the data output nodes corresponding to sensors 22-1, 22-2, and 52-2 are shown.

in relative humidity between the two sensors and accurately reproduce the rate of relative humidity rise in sensor 22-2 and 52-2. The experimental data for sensor 52-1 is thought to be an experimental error caused by a potential preferential fluid pathway, as they were expected to produce similar relative humidity profiles as a result of the equal technological void distance at this height within the sample. Consequently, the 2D slice cross-section model is compared to the sensors at 0.22 m length to investigate the dissymmetry caused by the technological void.

The calibrated model under-predicts the relative humidity at sensor 22-1 and 22-2 as a result of the calibration to RH52-2 and the initial estimate of relative humidity. The greater under prediction in sensor 22-1 is expected as the technological void is smallest here and the hydration from the end would likely have a contribution to the relative humidity recorded in this location. Figure 7.9 also shows a comparison with the axisymmetric model results and indicates a good agreement between the models even though they assume different thicknesses for the technological void. An explanation for this is that the lag in the onset of hydration from both ends in the experiment delays the relative humidity uptake in the axisymmetric model but this is not the case for the radial hydration seen in the 2D slice cross-section. After *c.*220 days the relative humidity in the 2D slice cross-section begins to plateau. This is caused by the redistribution of suction within the model as the hydration source ceases; no more water enters the sample and so the internal pressure gradients seek to equilibrate. The resulting divergence of the axisymmetric and 2D slice cross-section relative humidity results for sensor 22-1 is caused by the 2D slice cross-section model not accounting for the hydration from each end of the sample. This divergence occurs in the results at *c.*250 days which suggests that the effect of the hydration from both ends is not significant until this time. However, this temporal prediction considers the location of the 2D slice cross-section to be at 0.6 m along the length of

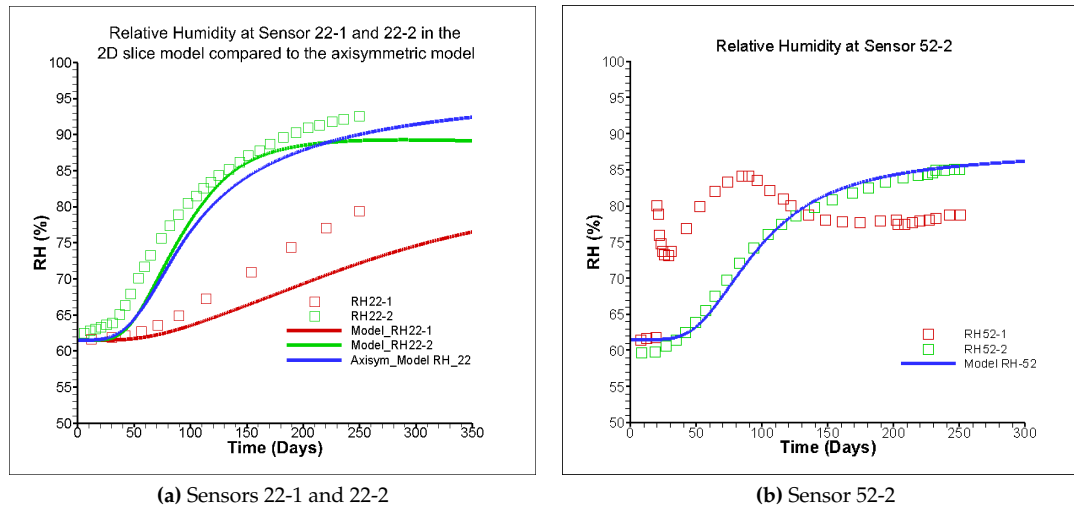


Figure 7.9: A comparison of the relative humidity results calculated with the axisymmetric and 2D slice cross-section models in sensors 22-1 and 22-2 (a). The axisymmetric model provides a good fit to the experimental data for sensor 22-2 but cannot recreate the dissymmetry with sensor 22-1. However, the 2D slice cross-section model creates this dissymmetry if the boundary conditions include hydraulic shut down when the technological void is filled, but eventually under predicts the relative humidity values because hydration from the sample ends is not considered. Sensor 22-2 is under predicted because the 2D slice cross-section model does not include hydration from the sample ends, which would likely affect the relative humidity data at 0.22 m along the core. The 2D slice cross-section model also provides a good fit to sensor 52-2 (b).

the core and it would be reasonable to expect to see this divergence earlier if the slice were at 0.22 m.

In order to investigate the hydraulic contribution of the host rock the 2D slice cross-section model was run with constant hydration through the radial boundary. The relative humidity calculated from this model is presented in Figure 7.10. The model calculates a good agreement to sensor 22-2 although predicts a higher final relative humidity. However, the same relative humidity results are predicted for sensor 22-1 and 52-2 (Figure 7.10b) which indicates that this hydraulic contribution from the host rock results in an over prediction at these sensor locations. In addition, the dissymmetry in relative humidity is not reproduced if a constant hydration source is modelled.

7.4.2 Axial stress

Axial stress calculated by the NLE model is presented in Figure 7.11(a). The development of stress matches well the trend of the experimental results recorded for the sensor at 0.00 m and calculates the final stress to within 0.4 MPa after 250 days. The rate of stress build up is very similar to that measured during the experimental results up until *c.*180 days, after which the experimental results plateau. The influence of the closure of the technological void can be seen in the model results; the change in gradient at *c.*57 days corresponds to the time at which the technological void becomes fully closed in the model.

There exists a very small difference in the stress calculated at each end which is due to mesh dependencies in the mechanical solution. As the material deforms any differences in strain in the element from which the stress is determined are reflected in the final stress calculation.

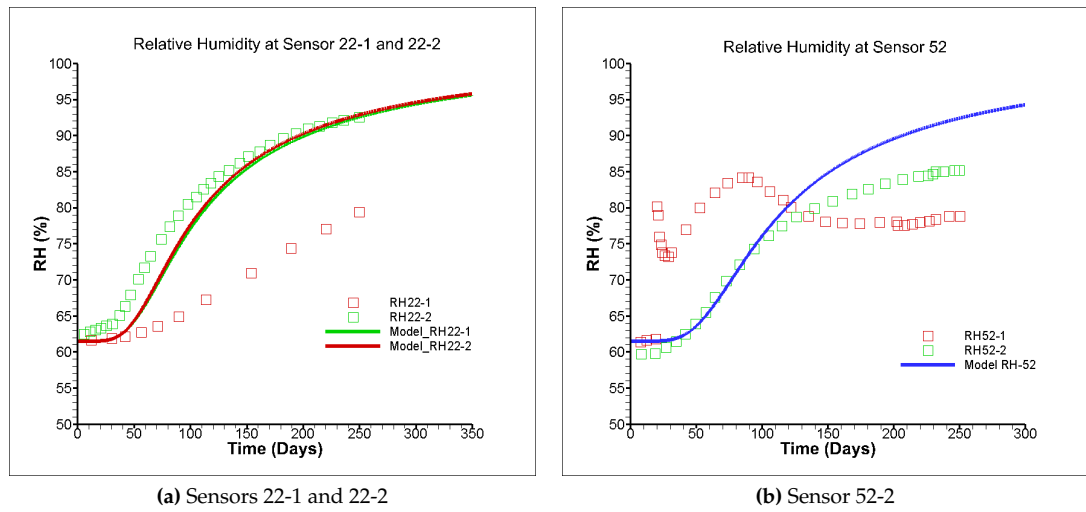


Figure 7.10: Model results for a 2D slice cross-section simulation in which the hydraulic boundary is not turned off once the technological void is filled. The results show a reasonable match to the relative humidity virtually no difference between the two sensor locations for sensors 22-1 and 22-2. Furthermore, the final relative humidity is over predicted for sensor 52-2.

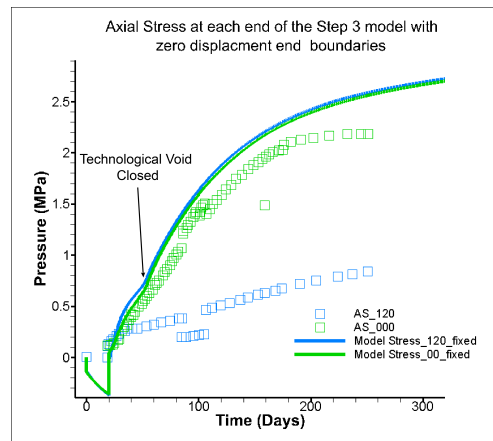


Figure 7.11: Model results compared to the measured axial stress. The stress accumulation follows the experimental data and calculates a final axial stress to within 0.3 MPa of the data for the sensor at 0.00 m. However, the time lag in hydration from the ends of the sample results in a tensile stress forming at the ends of the sample

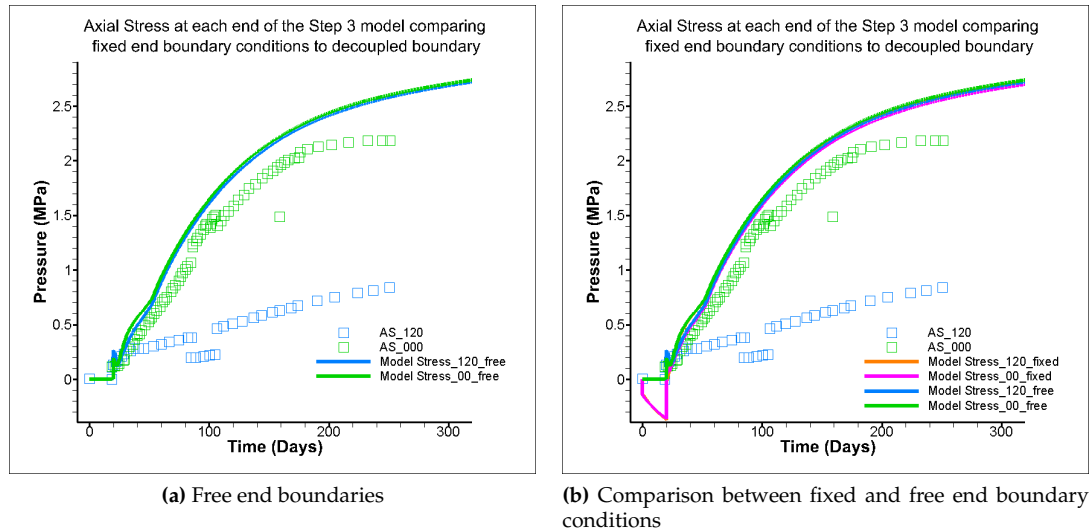


Figure 7.12: (a) Axial stress development calculated with a decoupled mechanical boundary with an expansion limit of 0.1 mm at each end. The tensile stress seen in Figure 7.11 does not build up because the end mechanical boundary is not fixed. (b) A comparison between the axial stress calculated with a decoupled end boundary condition and a fixed boundary condition. The results are almost identical suggesting that the development of the tensile stress is caused by the fixed end boundary condition.

However, the difference in the stress calculated at each end is less than 1% of the final stress.

Figure 7.11 includes the evolution of axial stress during the first 20 days. The model predicts a development of tensile stress. This indicates that the zero displacement boundary at the ends of the sample may not be valid. One possible explanation for this is that there may be some movement of the plug at the edge of the sample where hydration is occurring that causes a separation between the centre of the sample and the plug during the initial hydration of the edge.

Figure 7.12 shows the development of axial stress when the end boundary conditions are allowed to expand up to 0.1 mm but contract freely i.e. a decoupled mechanical boundary with an expansion limit. The results indicate that the tensile stresses are not developed as the centre of the sample is able to contract at the same time that the outer area of the sample expands. This follows as a result of the elastic assumption controlled the Poisson's ratio of the sample controls the amount of axial deformation for a given transverse strain. The deformation is shown in Figure 7.13 as the moving mesh deforms during the initial hydration stages. The jump in axial stress followed by reduction and subsequent increase in Figure 7.12 after c.20 days is due to the application of the hydraulic boundary conditions and is likely a numerical error caused by the rapid change from 64 MPa suction to 0.1 MPa suction over a course of a few minutes i.e. turning on the hydration source. However, the displacement of the end boundaries indicates that the sample is not in contact with the plug until the second rise in axial stress. As the development of swelling pressure of interest is against the plug and the drift excavation, the axial stress before contact can be discounted. To test this assumption Figure 7.12b plots the axial stress calculated with decoupled boundary conditions against the fixed end boundary conditions. The results are almost identical after contact is made suggesting that it is acceptable to present the axial stress results with a zero swelling pressure assumed until contact of the pressure sensor and the plug has occurred (Figure 7.14).

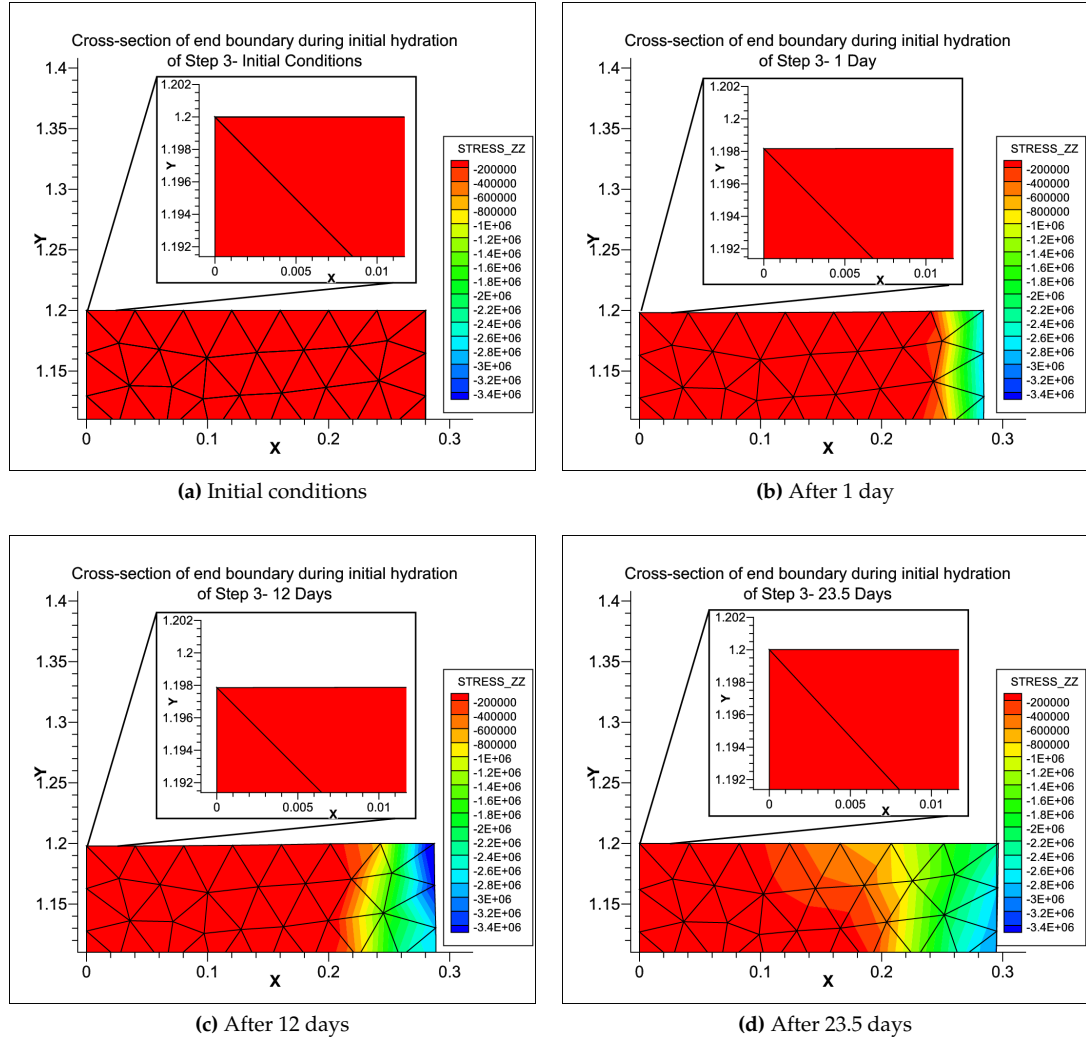


Figure 7.13: The evolution of the end of the core in a model that accommodates up to 1 mm axial deformation i.e. a free axial boundary. After 1 day the centre of the sample has contracted in response to the increase in lateral swelling at the hydrating edge. This deformation increases after 12 days. End hydration begins after c.20 days [Wang, 2012] leading to axial expansion and contact after 23.5 days.

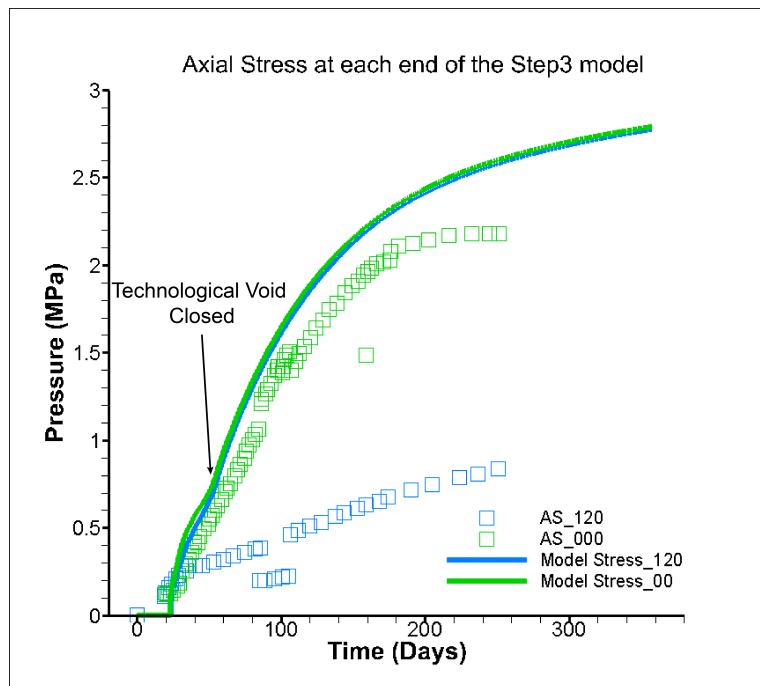


Figure 7.14: Axial stress development calculated with a model decoupled mechanical boundary at each end and only considering axial stress development to begin once the pressure sensor is in contact with the end plugs.

Unfortunately experimental data is only recorded for the initial conditions and after *c.*20 days. As a result, there are no data that can be used to test this hypothesis or indicate that an alternative process may be occurring e.g. plastic deformation at the edges that corresponds to no stress change at the pressure sensor.

7.4.3 Radial stress

In the axisymmetric model radial stress corresponds to the stress in the x axis direction. Due to the uniform technological void description in the axisymmetric model the calculation of the radial stress can only be considered to be an average value of the system. Figure 7.15(a) shows the model calculation compared to all three stress sensors. The results plot within the range of all three sensors and show a similar stress behaviour to that of sensor 60-3, suggesting that the difference in stress build up between the three sensors is caused by a difference in thickness of technological void.

The experimental data indicate that the technological void is filled at sensors 60-1 and 60-3 after *c.*20 days but the axisymmetric model predicts a technological void closure after *c.*57 days. This is consistent with both the slower than experiment closure rate in the Step 2 model results and the geometry difference of the void as represented by the axisymmetric model compared to the reality of the experiment.

The 2D plane strain slice cross-section model accounts for the non-symmetric technological void and, due to the geometric set up of the model, the stress in the y axis corresponds to the radial stress at sensor 60-2. The model calculation is shown in Figure 7.15(b) and indicates that the rate of stress accumulation after void closure is similar to that of the experimental results.

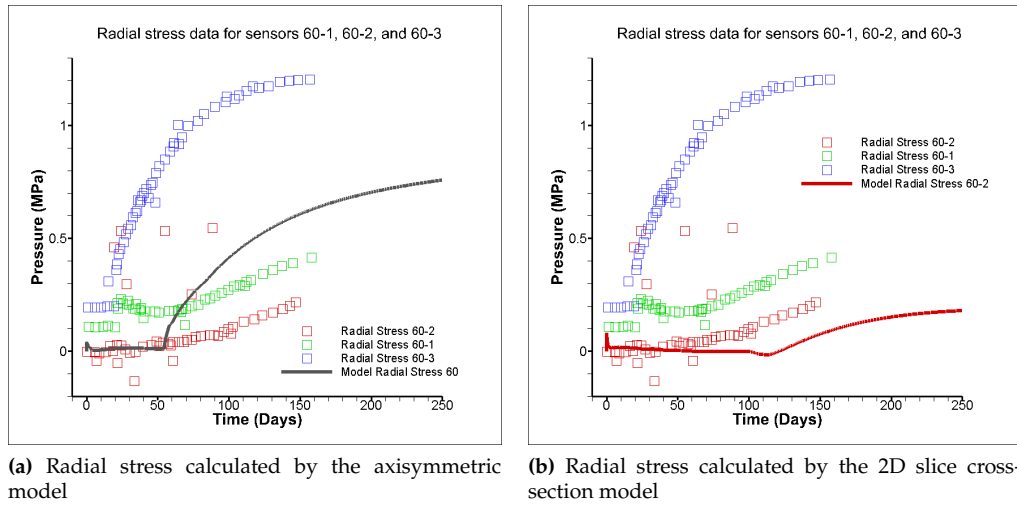


Figure 7.15: A comparison of the radial stress calculated for sensor 60-2 in the axisymmetric (a) and 2D slice cross-section (b) models. The axisymmetric model provides an average result that fall within all three stress sensor results. A good agreement to the experimental data is achieved for the 2D slice cross-section model, although the experimental data indicate an earlier more gradual rise in radial stress likely due to the formation of gel in the technological void.

However, the experimental data show the technological void closes after approximately 50 days, and the model calculates closure to occur after *c.*100 days. This is less than twice the time for the closure of the technological void in the axisymmetric model, which is half the distance. The difference in the rate of expansion in the two models can be explained by the larger possible strain in the 2D slice cross-section model (into the larger void). The greater strain results in a lower stiffness material at the top of the sample that is able to expand more rapidly. The experimental data suggest that this effect is more pronounced than in the model, which is likely due to the development of a gel in the technological void that causes a more rapid closure of the void with a material of low mechanical strength [Saba et al., 2014, Wang, 2012]. Consequently, the rise in radial stress occurs earlier and is more gradual than that predicted by the model, which does not consider the formation of a gel.

7.5 Discussion

The hydro-mechanical conditions of the PT-A1 performance test experiment are restricted to the transition from unsaturated conditions with axial confinement and radial free swell conditions to constant volume confinement. However, there is additional complexity in the form of a non-symmetrical technological void. In this instance a 2D axisymmetrical model is not sufficient to reproduce the experimental results and is therefore supplemented by a 2D plane strain slice cross-section model that can simulate the effect of the non-symmetrical technological void. Using the NLE model of 8 mechanical parameters it is possible to simulate the experimental results and determine the main processes and controlling factors. These are summarised in Table 7.3.

7.5.1 Hydraulic model

The calibration parameter m_a is reduced which results in an increase in calculated intrinsic permeability. Although this is clearly an undesirable change to have to make to reproduce experimental results, there are a number of possible reasons for this change to be made. Firstly the permeability model used in Step 2 is calibrated to the infiltration test results of relative humidity at four sensors along the axis of the small scale sample. The hydration in that experiment proceeds purely from the base of the sample under constant volume conditions and as such the model is calibrated in a situation where free swell behaviour is not observed and the full range in dry density is not investigated. In fact, the lowest sensor suggests that the permeability model underestimates the rate of change of relative humidity at low suctions even under constant volume conditions. Relative humidity data was not collected in the Step 2 experiments so injected water volume was used as the metric to calibrate the HM coupled model. As such, the minor edit to the permeability model required to fit the relative humidity data may in fact represent the impact of the large technological void on the amount of gel that forms at the sample edge (which is not accounted for in the model) and the subsequently more rapid uptake of water into the sample.

A second possible consideration is that the bentonite blocks are prepared via uni-axial com-

Process	Controlling Factors
Water Uptake	Bentonite permeability Rate of expansion (filling of technological void) Development of confining stress
Axial stress evolution	Suction pressure within the sample Mechanical and Hydraulic stress states
Swelling into the void	Mechanical stiffness of the material Bentonite permeability

Table 7.3: Main controls on the hydro-mechanical behaviour during the PT-A1 performance test modelled with the NLE model

paction to the desired dry density (1.97 Mg/m^3) [Saba, 2014]. This could have created an alignment of the clay particles that may lead to a degree of anisotropy to the intrinsic permeability. The permeability model is initially calibrated to the infiltration test in Step 1 where data were collected for fluid flow parallel to the axis of compaction. In both Step 2 and Step 3 the presence of the technological void results in flow in the axis perpendicular to the axis of compaction which may have a slightly higher permeability.

Finally, the large scale of the experiment requires that the core is made up of a number of compacted bentonite-sand blocks. The contact between the blocks could therefore provide a potentially higher permeability zone and lead to a heterogeneous sample permeability. Even the self-sealing effect of bentonite would require some expansion of the blocks to fill the voids and seal the blocks, which would reduce the dry density and increase the permeability. Furthermore, the inclusion of the sensors within the blocks also represents potential voids that can lead to a reduced dry density and increased permeability in their local vicinity as the bentonite expands upon hydration. This is most evident in sensor 52-1 where the relative humidity profile increases very sharply after approximately 20 days before falling sharply up to c.40 days. This could be caused by the hydrating fluid reaching the sensor via a preferential pathway.

7.5.2 Effect of the technological void

The non-symmetric nature of the technological void has an impact on the final degree of homogeneity of the bentonite-sand core. As the permeability of the bentonite is porosity dependent, and therefore dry density dependent, the difference in strain and water content experienced by the hydrating core filling the non-symmetric void has an impact on the hydraulic properties of the hydraulic seal. This can be visualised in the results of the 2D slice cross-section model.

An expansive mechanical strain calculated in the solution leads to a reduction in dry density and material stiffness and an increase in permeability and porosity. This can be seen in Figure 7.16 which shows a series of porosity maps of the 2D slice cross-section model through time. The swelling of the core into the larger technological void at the top of the drift hole leads to an increase in porosity that evolves through the experiment. Initially the sample is assumed to have a constant porosity (Figure 7.16(a)), but this rapidly changes upon hydration from the technological void. Porosity increases at the edge of the sample as it expands to fill the void. Once the void is filled the edge material becomes consolidated by the further hydration and expansion of the centre of the sample, which leads to a reduction in porosity in this zone and a tendency towards homogenisation of the sample (Figure 7.16(d)).

The dry density of the sample is also dependent on the strain of the sample and shows a similar evolution of a reduction as expansion into the void occurs followed by a homogenisation once the void is filled (Figure 7.17).

Due to the porosity dependence of the permeability model of Liu et al. [2011] the non-symmetric technological void also influences the permeability of the sample. This is evident in Figure 7.18 and indicates that hydraulic flow initially is likely to be concentrated around the edges of the sample and, although the sample becomes more homogeneous with time, a higher permeability zone remains towards the top at the end of the experiment. This has implications for the design criteria and effectiveness of the hydraulic seal as a horizontal emplacement such as this is likely to produce areas of higher permeability due to the non-symmetric technological void. Typically design criteria work from the target dry density once the technological void

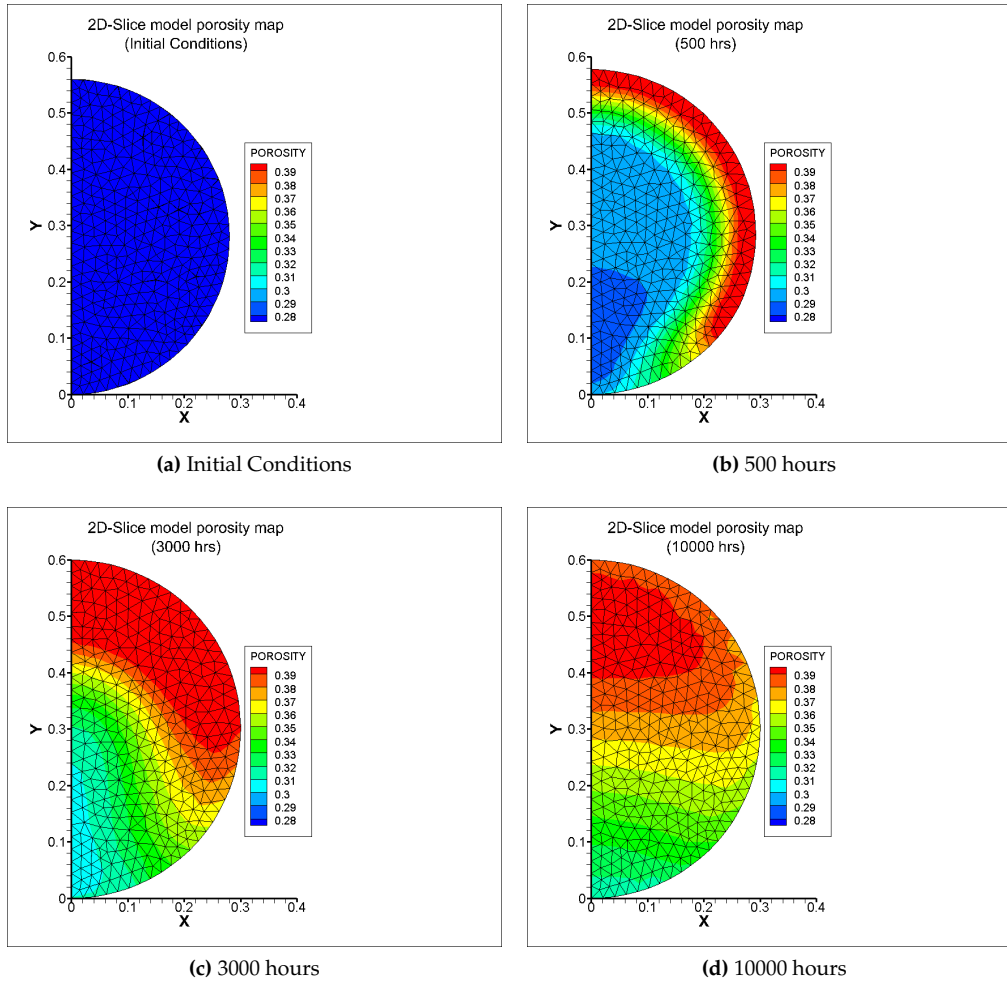


Figure 7.16: The evolution of porosity through time in the 2D slice cross-section model of Step3 from initial conditions (a) to the end of the simulation (d). The porosity evolves as a function of the deformation and therefore reflects the difference in hydraulic properties caused by the non-symmetric technological void. At the start of the simulation porosity increases at the edge of the sample as it expands into the void (b) and (c). Once the void is filled the further hydration of the centre of the sample causes compression of the material at the boundary and a subsequent decrease in porosity (d).

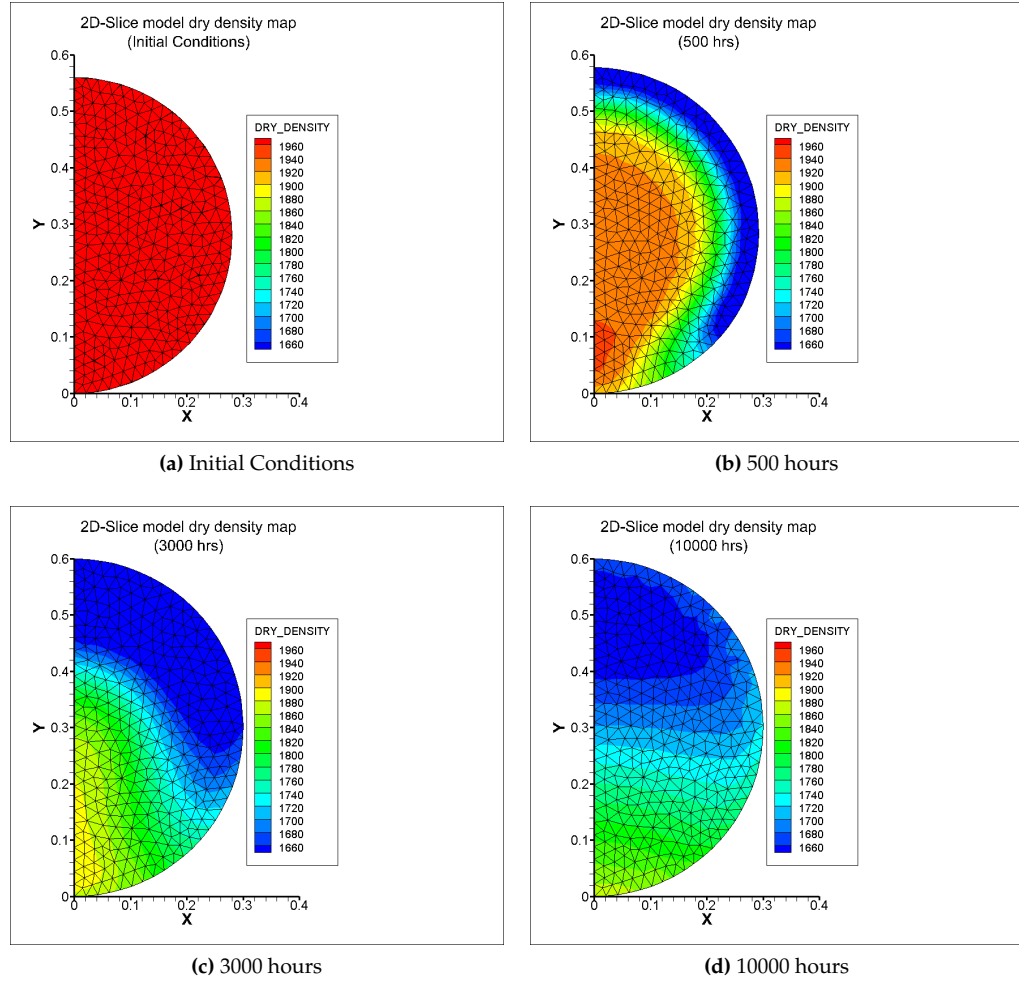


Figure 7.17: The evolution of dry density through time in the 2D slice cross-section model of Step3 from initial conditions (a) to the end of the simulation (d). The dry density evolves as a function of the deformation and impacts the hydraulic properties such as maximum saturation, that vary throughout the sample due to the non-symmetric technological void. At the start of the simulation dry density decreases at the edge of the sample as it expands into the void (b) and (c). Once the void is filled the further hydration of the centre of the sample causes compression of the material at the boundary and a subsequent increase in dry density as the sample tends towards homogenisation (d).

is filled as the final swelling pressure can be predicted by empirical relationships such as that proposed by Wang [2012]. In non-symmetric void scenarios the target dry density is therefore an average value for the total final volume of the core. This modelling of the non-symmetric technological void suggests that in the hydration process dry density, porosity, and permeability are not homogeneous throughout the hydraulic seal, and can therefore lead to hydraulic and mechanical heterogeneity. Although this 2D slice cross-section model does not consider the effect of the hydration from both ends of the sample there is a degree of homogenisation after 10000 hours that would likely be improved with axial hydration.

The model results for net mean stress evolution over time are presented in Figure 7.19. Mean stress rises at the edges of the sample in a similar distribution to the change in porosity, dry density, and permeability during the initial stages of hydration. A peak mean stress is reached as the sample edges are exposed to very low suctions during the flooding of the technological void, after which there is a reduction in peak mean stress but an increase in mean stress throughout the sample leading to a homogenisation of the mean stress field.

Consistent to all the results presented in Figures 7.16 to 7.19 is the heterogeneity induced by differential swelling into the non-symmetrical technological void. There exists a zone towards the top of the sample that maintains an elevated porosity and permeability, and a reduced dry density and net mean stress. This heterogeneity induced by the swelling from an initially homogeneous sample is an important consideration for designing future hydraulic seals and has been identified as an important area for further research. In some repository systems, such as the Swiss and Belgian concepts [Gens et al., 2013, NAGRA, 2009], experimental investigations have focussed on the behaviour of a bentonite block and pellet mixture to tend towards a homogeneous mixture. This is motivated by the desire to generate a material of consistent density with ease of emplacement i.e. pellets can be emplaced more easily into the remaining voids than compacted blocks. However, less attention has been paid to the possibility of generating heterogeneity from an initially homogeneous sample through differential swelling. The Engineered Barrier System (EBS) Task force project has begun to investigate the development of heterogeneity [Holton et al., 2012] through the swelling of bentonite into a void space [Dueck et al., 2011, 2014]. In small scale experiments with both directional and symmetrical void spaces and hydration sources Dueck et al. [2014] indicate the development of heterogeneity, especially with respect to the dry density and subsequent swelling pressure. Modelling of the SEALEX performance test PT-A1 suggests that this heterogeneity can be developed in full scale repository conditions and is therefore an important consideration for future research into hydraulic seals.

Bentonite homogenisation is often assumed as part of the design criteria and as such there is an increasing focus on understanding the process and developing numerical modelling tools. As recently as November 2015 at the 6th Implementing Geological Disposal of Radioactive Waste Technology Platform (IGD-TP) Exchange Forum a new project investigating bentonite homogenisation, named 'HomoBento', was put forward [www.igdtp.eu]. The Engineered Barrier experiment that has recently been dismantled at Mont Terri rock laboratory investigated the variation in dry density and porosity in a NAGRA specification full-scale test that included compacted bentonite blocks and pellets [NAGRA, 2009]. In addition to the EB experiment, experiments such as the Full Scale High Level Waste Engineered Barrier Experiment (FEBEX), Large Scale Sealing Experiment (NSC), KBS-3V 40% Scale Buffer demonstrations, and the PRA-CLAY experiment can all provide experimental data for model develop-

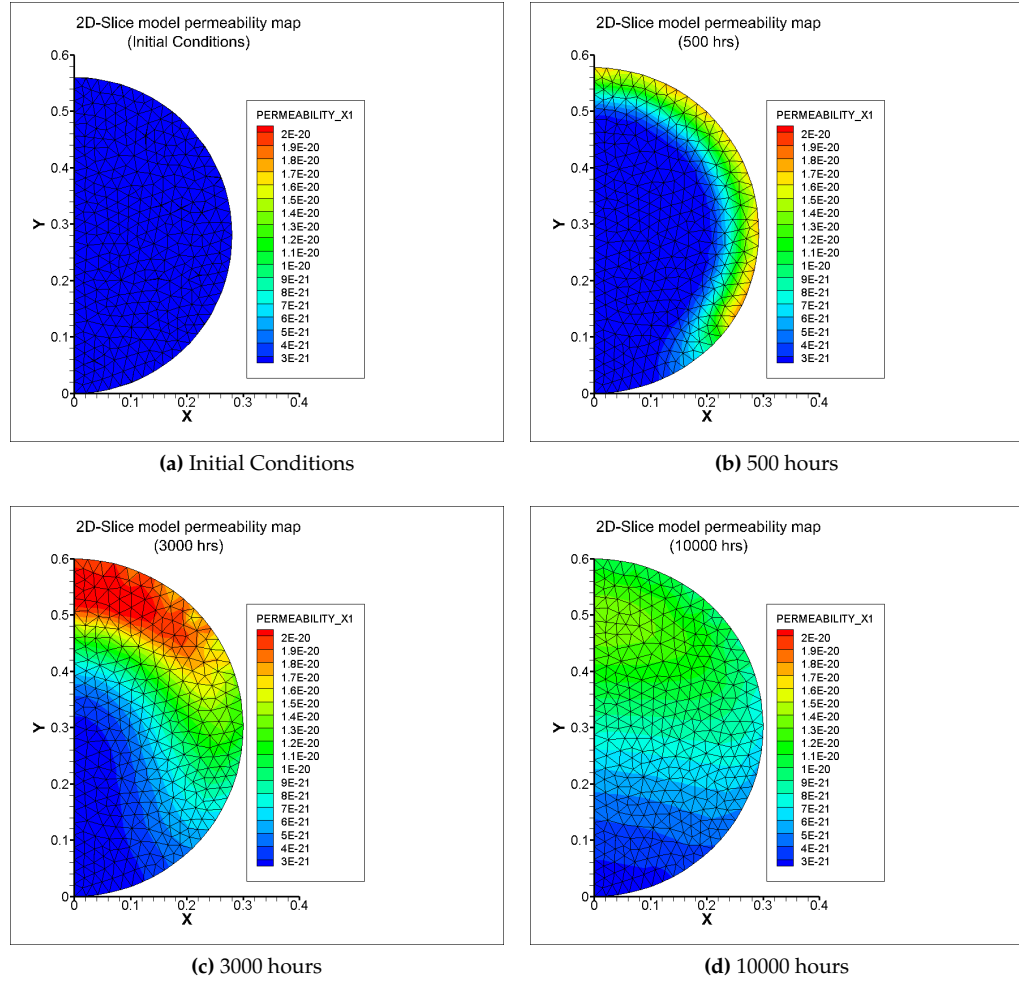


Figure 7.18: The evolution of permeability through time in the 2D slice cross-section model of Step3 from initial conditions (a) to the end of the simulation (d). The permeability model of Liu et al. [2011] implemented in this model is porosity dependent and therefore evolves as a function of the deformation. The non-symmetric technological void leads to a non-uniform permeability field. At the start of the simulation permeability increases at the edge of the sample as it expands into the void (b) and (c). Once the void is filled the hydration of the centre of the sample causes compression of the material at the boundary and a subsequent decrease in permeability as the sample tends towards homogenisation (d).

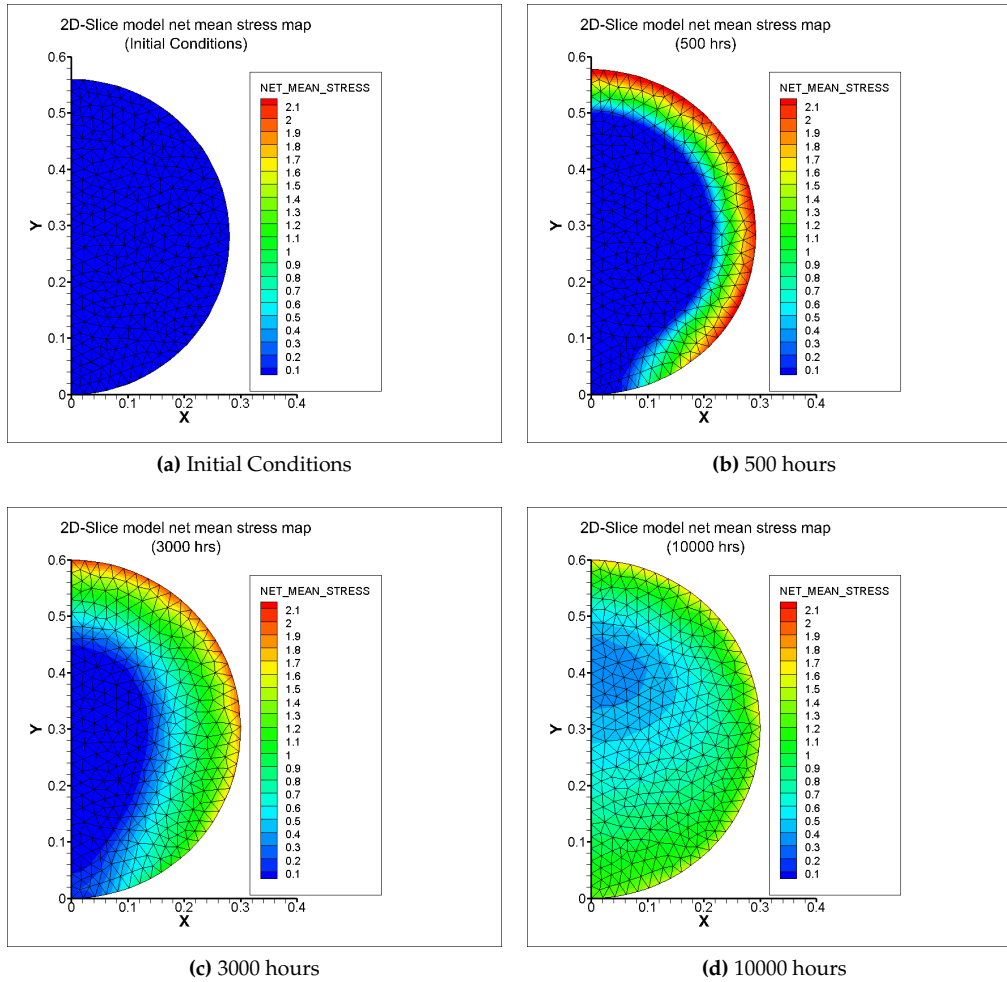


Figure 7.19: The evolution of net mean stress (p) through time in the 2D slice cross-section model of Step3 from initial conditions (a) to the end of the simulation (d). There is an initial peak in mean stress during the early stages of hydration around the edges of the sample. As the hydration front proceeds through the sample the mean stress rises following the same distribution as the hydrating fluid ((b) and (c)). Once the technological void is closed the net mean stress begins to tend towards a homogenised stress field (d).

ment and validation [www.igdtp.eu]. The EB and FEBEX experimental data have also been proposed to be used for the next phase of the DECOVALEX project (DECOVALEX-2019) in order to develop bentonite models that can predict the changes in hydraulic and mechanical properties as well as the degree of homogenisation through the experiment. With an extension to 3D and coupling to the thermal process this model could be used for this purpose.

7.5.3 Mechanical model

The NLE model without a source term to account for plastic collapse is used to model the behaviour of the PT-A1 experiment. The $1/10^{th}$ scale mock-up test of Step 2 there was evidence for the plastic collapse phenomenon that required specific consideration for modelling. However, the experimental results do not show the same behaviour in the PT-A1 Step 3 test. Wang [2012] suggest two possible reasons for this. Firstly, the increase in size of the sample leads to a reduction in the potential for plastic collapse to occur, and secondly, the location of the pressure sensor is different for the mock-up test and the full scale performance test. In the mock-up test the confining piston provided the means to measure the development of axial stress by controlling the load required to maintain constant volume conditions. As the swelling pressure developed an equivalent load was applied through the piston to prevent significant deformation. Similarly, during the plastic collapse process and axial stress reduction, the load applied was reduced. The change in the applied load defines the development of axial stress across the whole of the top surface of the sample [Lloret et al., 2003, Wang, 2012].

In contrast, the PT-A1 full scale experiment included two pressure sensors attached to the bentonite core in small recesses at each end [Wang, 2012]. These were located in the centre of the sample and therefore only collected data for the stress development at these discrete locations [Wang, 2012]. Therefore, it is possible that the plastic collapse phenomenon observed in the small scale mock-up test occurs in the PT-A1 experiment but the pressure sensors do not record the plastic deformation behaviour at their discrete locations.

The apparent lack of experimental data to support the presence of the plastic collapse phenomenon in the PT-A1 test has been observed in a previous full-scale *in situ* infiltration experiment: the isothermal test in Canada as modelled by Thomas et al. [2003]. Although this experiment was performed under the slightly different conditions of natural hydration and constant volume conditions, it nevertheless did not exhibit plastic deformation.

The experimental results also exhibit a dissymmetry in the stress development at each end of the sample under the same hydration conditions. As yet, there is no experimental explanation for this, although it is possible that the plug at 1.2 m experienced some deformation that accommodated some of the swelling pressure development, or bentonite extruded into unaccounted for voids. The model boundary conditions are equal at each end and therefore the NLE model calculates equal results for each end of the sample.

7.5.4 Implications for hydraulic seal design criteria

The NLE model for Step 3 provides an insight into the potential for a heterogeneous permeability and dry density to develop when a non-symmetrical technological void is present. This has implications for the potential hydraulic seal design where the swelling pressure and hydraulic properties are considered. Furthermore, the radial stress development may need to be considered in conjunction with the bedding orientation in a claystone host rock when

excavating the drift hole. For example, the lowest swelling pressure is generated where the technological void is greatest because more swelling occurs and the bentonite has a lower dry density and therefore can exert a lower swelling pressure [Wang, 2012]. A desirable property of bentonite is the development of a swelling pressure on the excavated walls of the drift or tunnel, and this is one of the main design criteria. The potential development of heterogeneous swelling pressures caused by a non-symmetrical technological void therefore may need to be considered in the design criteria, especially if the bedding orientation is conducive to spalling in the regions where the dry density will be lower than the design average.

Another main design criterion of a hydraulic seal is to provide a low permeability barrier between the waste and the geosphere [Arnold et al., 2011]. The modelling of the 2D slice cross-section suggests that expansion of bentonite into the non-symmetrical technological void causes an increase in permeability of up to an order of magnitude higher than initial conditions. However, as bentonite has a very low intrinsic permeability at the initial dry density at emplacement, this is still within the design criteria for a hydraulic seal such as those proposed by Arnold et al. [2011] for abandonment of deep borehole waste disposal.

The persistence of these induced heterogeneities can be visualised in Figure 7.20 where the net mean stress (swelling pressure), dry density, and permeability are shown for a model simulation extending to 11.5 years. The model calculations indicate that, even though the suction pressure has equilibrated throughout the sample (Figure 7.20d), the key metrics of swelling pressure, dry density, and permeability remain heterogeneous. The heterogeneous nature of the swelling pressure increases with time whereas the permeability has gradually equilibrated. The fluid transfer within the sample has led to a build up a swelling pressure at the base of the core due to the higher dry density in this region. This effect could potentially be reduced by hydration from each end of the sample but simulation of this would require a full 3D model, the development of which would be a potential area of future work.

7.6 Conclusions

The non-linear elastic model without the source term correction for plasticity is successfully applied to simulate the experimental results of the PT-A1 performance test. An axisymmetric model was combined with a 2D plane strain slice cross-section model to investigate the effect of a non-symmetrical technological void around the sample. A good agreement to the relative humidity data is achieved with a minor modification of the permeability model. The relative humidity results indicate that the hydraulic contribution from the host rock is negligible. Calculated axial and radial stresses also provide a good agreement to the experimental data, although the axial stress dissymmetry is not reproduced by the model. Modelling of the closure of the technological void over estimates the time it takes for the void to become filled, which is most likely due to the formation of a gel [Saba, 2014, Wang, 2012], which is not considered in the model. The geometry of the void has implications for the development of heterogeneity within the sample as the permeability, dry density (and therefore maximum swelling pressure), and mechanical stiffness are functions of the volume change as the bentonite expands to fill the void.

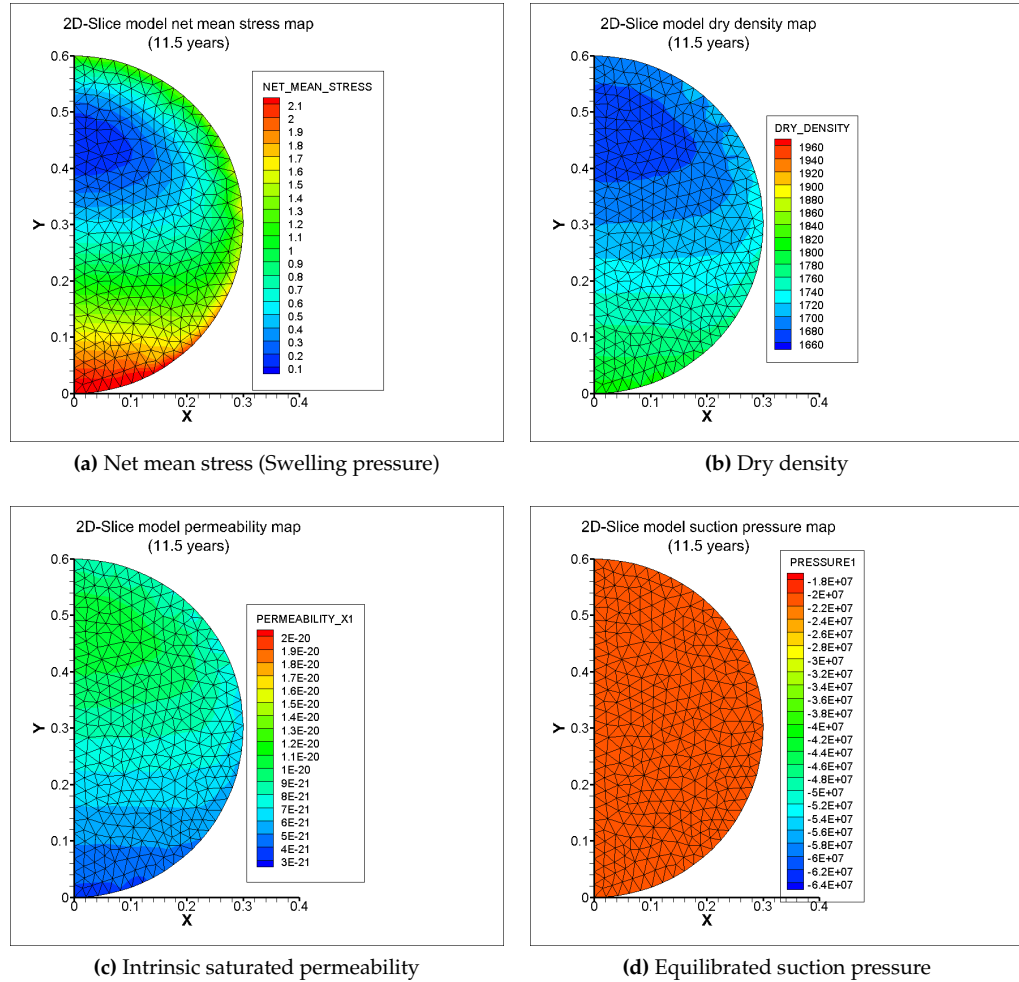


Figure 7.20: A comparison of the key metrics of net mean stress (swelling pressure), dry density, and permeability, along with the equilibrated suction pressure after approximately 11.5 years. The model predicts the persistence of the induced heterogeneity upon suction equilibration.

Chapter 8

Conclusions

The aim of this thesis was to develop a coupled process model that is able to reproduce the hydro-mechanical (HM) behaviour of bentonite under a variety of stress conditions with as simple a constitutive model and as few parameters as possible. In order to achieve this an HM coupled process model based on Richards' equation for unsaturated flow and strain-dependent non-linear elasticity has been developed and implemented in the open source code OpenGeoSys. A Lagrangian moving mesh has also been implemented to inform the material non-linearity associated with strains occurring as bentonite is hydrated and/or consolidated. The model was successfully applied to a series of experiments increasing in both scale and complexity from standardised laboratory tests, to a full scale *in situ* hydraulic seal performance test.

8.1 Developments in OpenGeoSys

Significant developments have been undertaken to extend the capabilities of the original code for the application of this model to the simulation of hydrating bentonite under a variety of conditions.

A major development is the implementation of a Lagrangian moving mesh (with respect to the mechanical process) and its use in informing the material non-linearity in the developed non-linear elastic mechanical model. The coupling mechanism between the hydraulic and mechanical processes was extended to be dependent on the mean stress and an explicit iterative procedure was employed. In addition, the hydraulic and mechanical meshes are decoupled such that volume dependent variables in the hydraulic solution may be updated within iterations in order to maintain consistency of volumetric variables within the hydro-mechanical process.

Within the hydraulic process, the key developments focussed on the implementation of the Dueck suction concept that directly couples the confining stress to the water retention properties. Furthermore, bentonite specific material models, including the implementation of a variety of permeability models and an enhancement of the Richards' equation implementation to utilise water content-suction data, were developed.

Development of the mechanical process focussed on the implementation of the strain-dependent non-linear elastic model that allows for non-recoverable strains in consolidation. The hydraulic contribution to the mechanical deformation or stress development is incorpo-

rated via a coupling term, known as the 'internal strain factor'. This represents both the double structure of bentonite via the swelling of aggregates into the macro porosity, and the transition from crystalline swelling to osmotic swelling.

Displacement dependent boundary conditions utilising the moving mesh application were developed for both the hydraulic and mechanical processes and for axisymmetric and 2D plane strain models. These provided a simple method of modelling the technological voids without the further computational cost of modelling the surrounding host rock.

Finally, the moving mesh application has been employed to define element variables dependent on element volume i.e. porosity, dry density, void ratio, and Young's modulus. These are used within the hydraulic and mechanical solutions and model output has also been developed to enable the visualisation of these key parameters in the results.

8.2 Findings

The standardised laboratory tests formed a parameterisation data set to which the developed model was calibrated. The coupled model was able to provide an adequate fit for consolidation at different suctions, and constant volume infiltration with a model of just 8 mechanical parameters, 4 hydraulic parameters, and one coupling parameter.

The permeability model proposed by Liu et al. [2011] was implemented and successfully calibrated to two separate bentonite infiltration tests. The coupling mechanism of Dueck suction, using the free swell suction curve and net mean stress to determine water retention properties under a range of degrees of confinement, was validated against a constant volume water retention test to show the applicability of the model.

The model was then applied to a $1/10^{th}$ scale mock-up test that contained a symmetrical technological void and three phases of changing stress conditions. Displacement dependent boundary conditions were developed and combined with the Lagrangian moving mesh to give an estimate of the rate of closure of the technological void.

Due to the observed wetting-induced collapse behaviour during Phase 1, the non-linear elastic model was extended to include a failure curve similar in definition to the loading-collapse curve in elasto-plastic models, that was combined with an applied source term to account for the collapse behaviour. This NLE-ST model was able to reproduce the axial stress development and water up-take data, and a comparison between the NLE and NLE-ST models with the same parameter set is able to provide an estimate of the energy dissipated through the sample during the collapse behaviour. However, the both the NLE and NLE-ST models over predict the elastic rebound upon confinement release in Phase 2a and 2b as the elastic strain energy remains in the sample.

A full scale *in situ* performance test (PT-A1) with a non-symmetrical technological void was then simulated with the non-linear elastic model without accounting for wetting-induced collapse. Displacement dependent boundary conditions were applied to a 2D axisymmetric model and developed for a 2D slice model to investigate the effect of the non-symmetric technological void. A minor adjustment to the permeability function provided an excellent fit to the experimental data if the boundary conditions simulated no contribution to the hydration from the host rock.

Simulation of the full scale *in situ* experiment has led to the following conclusions relevant to hydraulic seals:

- With a flooded technological void, a bentonite plug can swell to fill a technological void over relatively short time scales (a matter of weeks).
- Bentonite provides a very low permeability barrier to advective flow with a maximum simulated saturated intrinsic permeability on the order of $2 \times 10^{-20} \text{ m}^2$.
- A swelling pressure develops over the course of hydration which could act to support the excavated drift hole. This is dependent on the dry density and hydration state of the sample.
- Final dry density distribution is dependent on the diameter of the technological void. The design criteria of 1.67 Mg/m^3 dry density represents an average dry density for the whole sample. This may be applicable if the void is symmetrical, but the range of heterogeneity with respect to dry density (and consequently the final swelling pressure) is greater, and non-uniform, if the technological void is not symmetrical.
- A non-symmetrical technological void has the potential to induce heterogeneity within the sample with respect to dry density, swelling pressure, permeability, and material stiffness that may persist years after the technological void is filled. However, there remain some unexplained heterogeneities with respect to the axial swelling pressure.

The three main modelling steps have covered a range of hydro-mechanical conditions from which it is possible to identify key measurable metrics that can provide insight into the overall behaviour. These are:

- the suction pressure,
- the confining stress conditions i.e. the swelling pressure, and
- the dry density.

The suction pressure and confining stress conditions are combined to give the stress dependent water retention properties and the role of suction in the swelling behaviour of bentonite. These provide the key parameters for modelling the strongly coupled hydro-mechanical process of bentonite saturation. The dry density is directly related to the porosity and volume change associated with expansion or consolidation and is a key control on the development of swelling pressure. Furthermore, it is directly linked to the saturated intrinsic permeability and so knowledge of the dry density can provide a significant insight into the material characteristics.

8.2.1 Recommendations for hydraulic seal design

The key design criteria for hydraulic seals are the capacity of the bentonite to swell into a technological void, the ability to provide a low permeability seal for advective flow, and the capacity to provide a swelling pressure to support the excavation. This work confirms the potential for bentonite to quickly expand and seal voids, and provide a low permeability barrier. However, it also highlights the impact of a horizontal, or sub-horizontal, emplacement method for the hydraulic seal as hypothesised by the French disposal programme [ANDRA, 2005].

The design swelling pressure is calculated as a function of the target average dry density. Model simulations indicate that the non-symmetrical void results in a degree of persistent heterogeneity in dry density which, in turn, causes heterogeneity of swelling pressure development. This has been observed in other long term full scale *in situ* experimental programmes such as the Engineered Barrier (EB) test and Full-scale High Level Waste Engineered Barrier Experiment (FEBEX), where heterogeneity exists within a bentonite buffer system after more than a decade [NAGRA, 2009]. The full scale performance test PT-A1 in the Tournemire argillite indicated the lack of contribution of the host rock to the hydration of the bentonite core- modelling of the relative humidity data supported the hypothesis that hydration proceeded from the flooded technological void and the porous stones in the plugs only. Therefore, based on these results, the following considerations are recommended for hydraulic seal design:

- Reduce the size of the technological void in a horizontal emplacement method if possible. If a homogeneous swelling pressure is desired, a smaller technological void would ensure that the emplaced core is closer to the target average dry density by reducing the induced heterogeneity.
- An alternative measure could be to backfill the remaining void with bentonite pellets of a similar dry density as proposed in the NAGRA high level waste concept [NAGRA, 2009].
- Artificially hydrate the seal before closure. The lack of hydration from the host rock suggests that these seals require artificial hydration in order to fill the technological void over short time-scales and provide the structural support given by the development of swelling pressure.

8.3 Future Research

The model developed in this work is able to reproduce many aspects of the experimental results at different scales. However, there are a number of areas in which the model could be further developed for future use. These include:

- Incorporating a mechanism by which energy can be dissipated within the system. While there has been significant effort to keep the number of independent parameters to a minimum by using a non-linear elastic approach, it may be pertinent in future developments of the model to include a mechanism for energy dissipation. This could be achieved by incorporating plasticity into the mechanical model.
- Specific consideration of the micro and macro structural scales and the ratios between the two. Within the mechanical framework the internal strain factor used in this model could provide a means to incorporate the interaction between the micro and macro structural scales in future developments.
- Incorporation of a representation of gel formation in the technological void.
- Anisotropy of the permeability model could be investigated.

- The permeability model could be developed to include a parameter for the exfoliation of clay aggregates at low suctions in line with the interpretation of Wang [2012]. This may allow the rapid hydration of the infiltration test in Wang [2012] and the step jump in hydration in Ye et al. [2009] to be modelled.
- A consideration of hydraulic hysteresis caused by wetting and drying paths could also be considered if the model was to be used to model a scenario in which these two hydraulic stress paths are likely e.g. in a non-isothermal environment such as a buffer.
- Extension of the model to three dimensions. This would allow a better understanding of the persistence of the heterogeneity developed in the full scale performance test with a non-symmetrical technological void.

8.4 Summary

In summary, a strain dependent non-linear elastic mechanical model has been successfully implemented in OpenGeoSys and coupled to Richards' equation for unsaturated fluid flow. Significant code developments have included the implementation of a moving mesh to inform material non-linearity in the mechanical model. This fully coupled HM model has been successfully applied to a series of laboratory and full scale *in situ* experiments, allowing a better understanding of the development of heterogeneity within a sample as a result of differential swelling.

Bibliography

- G. Achari, R. C. Joshi, L. R. Bentley, and S. Chatterji. Prediction of the hydraulic conductivity of clays using the electric double layer theory. *Canadian Geotechnical Journal*, 36(5):783–792, 1999. ISSN 0008-3674. doi: 10.1139/t99-052.
- Setianto Samingan Agus. *An Experimental Study on Hydrodynamic Characteristics of Compacted Bentonite-Sand Mixtures*. PhD thesis, 2005.
- Setianto Samingan Agus, Tom Schanz, and Delwyn G. Fredlund. Measurements of suction versus water content for bentonite-sand mixtures. *Canadian Geotechnical Journal*, 47(5):583–594, 2010. ISSN 0008-3674. doi: 10.1139/T09-120.
- Setianto Samingan Agus, Yulian Firmiana Arifin, Snehasis Tripathy, and Tom Schanz. Swelling pressure-suction relationship of heavily compacted bentonite-sand mixtures. *Acta Geotechnica*, 8(2):155–165, 2012. ISSN 1861-1125. doi: 10.1007/s11440-012-0189-0.
- E. E. Alonso, A. Josa, and A. Gens. A constitutive model for partially saturated soils. *Géotechnique*, 40(3):405–430, 1990. ISSN 0016-8505. doi: 10.1680/geot.1990.40.3.405.
- E. E. Alonso, E. Romero, and C. Hoffmann. Hydromechanical behaviour of compacted granular expansive mixtures: experimental and constitutive study. *Geotechnique*, 61(4):329–344, 2011. ISSN 0016-8505.
- E.E. Alonso, J. Vaunat, and A. Gens. Modelling the mechanical behaviour of expansive clays. *Engineering Geology*, 54(1-2):173–183, 1999. ISSN 00137952. doi: 10.1016/S0013-7952(99)00079-4.
- E.E. Alonso, J. Alcoverro, F. Coste, L. Malinsky, V. Merrien-Soukatchoff, I. Kadiri, T. Nowak, H. Shao, T.S. S Nguyen, A.P.S. Selvadurai, G. Armand, S.R. R Sobolik, M. Itamura, C.M. M Stone, S.W. W Webb, A. Rejeb, M. Tijani, Z. Maouche, A. Kobayashi, H. Kurikami, A. Ito, Y. Sugita, M Chijimatsu, L. Börgesson, J. Hernelind, J. Rutqvist, C.-F. Tsang, P. Jussila, and a.P.S. Selvadurai. The FEBEX benchmark test: case definition and comparison of modelling approaches. *International Journal of Rock Mechanics and Mining Sciences*, 42(5-6):611–638, 2005. ISSN 13651609. doi: 10.1016/j.ijrmms.2005.03.004.
- ANDRA. Dossier 2005 Argile- Evaluation of the feasibility of a geological repository in an argillaceous formation. Technical report, 2005.
- Pe Anttila, Jorma Autio, Jarno Berghäll, Lennart Börgesson, Magnus Eriksson, Annika Hagros, Bo Halvarsson, Erik Johansson, Raimo Kotola, and Ilpo Parkkinen. KBS-3H Design Description 2007. Technical Report POSIVA 2008-01, POSIVA OY, 2008.

-
- B. Arnold, P. Brady, P. Vaughn, and S.A. Orrell. Reference design and operations for deep borehole disposal of high-level radioactive waste. Technical Report SAND2011-6749, 2011.
- Laura Asensio. *Hydro-mechanical elastoplastic model of expansive bentonite behaviour in free swelling conditions*. PhD thesis, 2013.
- Wiebke Baille, Snehasis Tripathy, and Tom Schanz. Swelling pressures and one-dimensional compressibility behaviour of bentonite at large pressures. *Applied Clay Science*, 48(3):324–333, 2010. ISSN 01691317. doi: 10.1016/j.clay.2010.01.002.
- J D Barnichon, P Dick, and C Bauer. The SEALEX in situ experiments : Performance tests of repository seals. In *Harmonising Rock Engineering and the Environment*. 2012. ISBN 9780415804448.
- Maurice A Biot. GENERAL THEORY OF THREE-DIMENSIONAL CONSOLIDATION. *Journal of Applied Physics*, 12(2):155–164, 1941.
- J. T. Birkholzer and Y. W. Tsang. Modeling the thermal-hydrologic processes in a large-scale underground heater test in partially saturated fractured tuff. *Water Resources Research*, 36(6): 1431–1447, feb 2000. ISSN 00431397. doi: 10.1029/2000WR900025.
- James A. Blatz, Yu-Jun Cui, and Luciano Oldecop. Vapour Equilibrium and Osmotic Technique for Suction Control. *Geotechnical and Geological Engineering*, 26(6):661–673, 2008. ISSN 0960-3182. doi: 10.1007/s10706-008-9196-1.
- Gabriella Bolzon and Bernhard A Schrefler. State Surfaces of Partially Saturated Soils: An Effective Pressure Approach. *Applied Mechanics Reviews*, 48(10):643–649, 1995. ISSN 00036900. doi: 10.1115/1.3005044.
- A. Bond, K. Thatcher, N. Chittenden, C. McDermott, and A. Fraser-Harris. Rwm coupled processes project: First annual report for rwm participation in decovalex-2015 tasks a and c1. amec report 18040-tr-002 v2.1. Technical report, 2014.
- A.E. Bond and S.J. Benbow. QPAC Multi-Phase Flow Module Functional Specification and Architectural Design. Quintessa Report QRS-QPAC-HYD-2 v1.0. Technical report, 2009.
- L. Börgesson, Torbjörn Sanden, Lars-Erik Johannesson, and J. Hernelind. Modelling of the physical behaviour of water saturated clay barriers. Laboratory tests, material models and finite element application. Technical report, SKB, 1995.
- RI Ronaldo I Borja and SR R Lee. Cam-clay plasticity, part 1: implicit integration of elastoplastic constitutive relations. *Computer Methods in Applied Mechanics and Engineering*, 78: 49–72, 1990.
- Michael H Bradbury and Bart Baeyens. Porewater chemistry in compacted re-saturated MX-80 bentonite. *Journal of contaminant hydrology*, 61(1-4):329–38, 2003. ISSN 0169-7722. doi: 10.1016/S0169-7722(02)00125-0.
- Wernt Brewitz and Tilmann Rothfuchs. Concepts and Technologies for Radioactive Waste Disposal in Rock Salt. 12:67–74, 2007.

-
- R.H. Brooks and T. Corey. Hydraulic properties of porous media. *Colorado State University Hydrology papers*, 3, 1964.
- M. A. Celia, E. T. Bouloutas, and R. L. Zarba. A general mass-conservative numerical solution for the unsaturated flow equation. *Water Resources Research*, 26(7):1483–1496, 1990. ISSN 00431397. doi: 10.1029/90WR00196.
- Johan Christian Clausen. *Efficient Non-Linear Finite Element Implementation of Elasto-Plasticity for Geotechnical Problems*. PhD thesis, Aalborg University, 2007.
- R F Craig. *Craig's Soil Mechanics. - 7th Edition*. Spon Press, 2004.
- D Croney, J.D. Coleman, and V.P.M Black. Movement and distribution of water in soil in relation to highway design and performance. Technical report, Highway Research Board Special Report no 40, 1958.
- Y.J J Cui, P Delage, and M Yahia-Aissa. A model for the volume change behavior of heavily compacted swelling clays. *Engineering Geology*, 64(2-3):233–250, 2002. ISSN 00137952. doi: 10.1016/S0013-7952(01)00113-2.
- G. de Marsily. *Quantative hydrogeology: Groundwater hydrology for engineers*. Academic Press, 1986.
- W. A. Deer, R. A. Howie, and J. Zussman. *An introduction to the rock-forming minerals. - 2nd Edition*. Pearson Prentice Hall, 1992. ISBN 978-0-582-30094-1.
- Pierre Delage and Yu Jun Cui. An evaluation of the osmotic method of controlling suction. *Geomechanics and Geoengineering*, 3(1):1–11, 2008. ISSN 1748-6025. doi: 10.1080/17486020701868379.
- J. Donea, A. Huerta, J. Ph Ponthot, and A Rodríguez-Ferran. Arbitrary Lagrangian Eulerian Methods. In *Encyclopedia of Computational Mechanics*, pages 1–25. 1999. ISBN 0470846992. doi: 10.1002/0470091355.ecm009.
- F. D’Onza, D. Gallipoli, S. Wheeler, F. Casini, J. Vaunat, N. Khalili, L. Laloui, C. Mancuso, D. Mašín, M. Nuth, J.M. Pereira, and R. Vassallo. Benchmark of constitutive models for unsaturated soils. *Géotechnique*, 61(4):283–302, 2011. ISSN 0016-8505. doi: 10.1680/geot.2011.61.4.283.
- Ann Dueck. *Hydro-mechanical properties of a water unsaturated sodium bentonite*. PhD thesis, Lund University, 2004.
- Ann Dueck. Laboratory results from hydro-mechanical tests on a water unsaturated bentonite. *Engineering Geology*, 97(1-2):15–24, 2008. ISSN 00137952. doi: 10.1016/j.enggeo.2007.11.001.
- Ann Dueck and Lennart Börjesson. Model suggested for an important part of the hydro-mechanical behaviour of a water unsaturated bentonite. *Engineering Geology*, 92(3-4):160–169, 2007. ISSN 00137952. doi: 10.1016/j.enggeo.2007.04.004.
- Ann Dueck, Reza Goudarzi, and Lennart Börjesson. TR-12-02 Buffer Homogenisation status report. Technical report, SKB, 2011.

-
- Ann Dueck, Reza Goudarzi, and Lennart Börgesson. TR-14-25 Buffer Homogenisation status report 2. Technical report, SKB, 2014.
- A Ferrari and A Seiphoori. Cyclic Water Retention Behaviour of Compacted Granular Bentonite. In *EAGE 2015*, pages 13–15, 2015.
- D. G. Fredlund, H. Rahardjo, and M.D. Fredlund. *Unsaturated Soil Mechanics in Engineering Practice*. John Wiley & Sons Ltd, 2012. ISBN 978-1-118-13359-0.
- Delwyn G. Fredlund and Norbert R. Morgenstern. Stress state variables for unsaturated soils. *Journal of the Geotechnical Engineering Division*, pages 447–466, 1977.
- D.G. Fredlund. Use of soil-water characteristic curve in the implementation of unsaturated soil mechanics. In *Third International Conference on Unsaturated Soils*, 2002.
- D.G. Fredlund and H. Rahardjo. *Soil mechanics for unsaturated soils*. John Wiley & Sons Ltd, 1993.
- D.G. Fredlund and Anqing Xing. Equations for the soil-water characteristic curve. *Canadian Geotechnical Journal*, 31(6):1026–1026, 1994. ISSN 0008-3674. doi: 10.1139/t94-120.
- D.A. Gallipoli, A. W. Bruno, F. D’Onza, and C. Mancuso. A bounding surface hysteretic water retention model for deformable soils. *Géotechnique*, 65(10):793–804, 2015. ISSN 17517656. doi: 10.1680/geot.14.P.118.
- Domenico. Gallipoli, S.J. Wheeler, and M. Karstunen. Modelling the variation of the degree of saturation in a deformable unsaturated soil. *Geotechnique*, 53:105–112, 2003.
- I. Gaus, P.L. Martin, E. Thurner, M. Vahanen, S-P. Teodori, F. Kober, and J-S. Kwon. FEBEX In Situ Test After 18 Years of Monitoring - Final Dismantling in 2015. In A. Schäfers and S. Fahland, editors, *International Conference on the Perforance of Engineered Barriers (PEBS). Physical and Chemical Properties, Behaviour & Evolution*, pages 97 – 102, 2014.
- A. Gens. Soil-environment interactions in geotechnical engineering. *Géotechnique*, 60(1):3–74, 2010. ISSN 0016-8505. doi: 10.1680/geot.9.P.109.
- A. Gens, M. Sánchez, B. Valleján, C. Imbert, M.V. Villar, and M. Van Geet. Hydromechanical behaviour of a heterogeneous compacted soil: experimental observations and modelling. *Géotechnique*, 61(5):367–386, 2011. ISSN 0016-8505. doi: 10.1680/geot.SIP11.P.015.
- A. Gens, B. Valleján, M.T. Zandarín, and M. Sánchez. Homogenization in clay barriers and seals: Two case studies. *Journal of Rock Mechanics and Geotechnical Engineering*, 5(3):191–199, 2013. ISSN 16747755. doi: 10.1016/j.jrmge.2013.04.003.
- Antonio Gens and E.E. Alonso. A framework for the behaviour of unsaturated expansive clays. *Canadian Geotechnical Journal*, 29:1013–1032, 1992.
- Antonio Gens, Marcelo Sánchez, and Daichao Sheng. On constitutive modelling of unsaturated soils. *Acta Geotechnica*, 1(3):137–147, 2006. ISSN 1861-1125. doi: 10.1007/s11440-006-0013-9.

-
- Christophe Geuzaine and Jean-François Remacle. Gmsh: A 3-D finite element mesh generator with built-in pre- and post-processing facilities. *International Journal for Numerical Methods in Engineering*, 79(11):1309–1331, 2009. ISSN 00295981. doi: 10.1002/nme.2579.
- Frank D Hansen and Christi D Leigh. Salt Disposal of Heat-Generating Nuclear Waste. Technical Report SAND2011-0161, SANDIA National Laboratories, 2011.
- R Helmig. *Multiphase flow and Transport Processes in the Subsurface. A contribution to the Modeling of Hydrosystems*. Springer- Verlag Berlin Heidelberg, 1997. ISBN 3-540-62703-0.
- Michael Holmboe, Susanna Wold, and Mats Jonsson. Porosity investigation of compacted bentonite using XRD profile modeling. *Journal of contaminant hydrology*, 128(1-4):19–32, 2012. ISSN 1873-6009. doi: 10.1016/j.jconhyd.2011.10.005.
- D. Holton, S. Baxter, and A. R. Hoch. Modelling coupled processes in bentonite: recent results from the UK’s contribution to the Äspö EBS Task Force. *Mineralogical Magazine*, 76(8):3033–3043, 2012. ISSN 0026461X. doi: 10.1180/minmag.2012.076.8.19.
- G.T Houlsby. The work input to an unsaturated granular material. *Geotechnique*, 47:193–196, 1997.
- Chongyu Hua. An inverse transformation for quadrilateral isoparametric elements: Analysis and application. *Finite Elements in Analysis and Design*, 7:159–166, 1990.
- J. Istok. *Groundwater modelling by the finite element method*. American Geophysical Union, 1989.
- A.C. Jacinto, M.V. Villar, and A Ledesma. Influence of water density on the water-retention curve of expansive clays. *Geotechnique*, 62(8):657–667, 2012.
- Bo Bengt Jönsson, Torbjörn Åkesson, Segad Meehdi, John Janiak, and Reine Wallenberg. Structure and forces in bentonite MX-80. Technical Report TR-09-06, SKB, 2009.
- O Karnland, S Olsson, and U Nilsson. Mineralogy and sealing properties of various bentonites and smectite-rich clay materials. Technical Report TR-06-30, SKB, 2006.
- D. Kavetski, P. Binning, and S.W. Sloan. Adaptive time stepping and error control in a mass conservative numerical solution of the mixed form of Richards equation. *Advances in Water Resources*, 24(6):595–605, 2001. ISSN 03091708. doi: 10.1016/S0309-1708(00)00076-2.
- Jin-Seop Kim, Sang-Ki Kwon, Marcelo Sanchez, and Gye-Chun Cho. Geological storage of high level nuclear waste. *KSCE Journal of Civil Engineering*, 15(4):721–737, 2011. ISSN 1226-7988. doi: 10.1007/s12205-011-0012-8.
- O. Kolditz, S. Bauer, L. Bilke, N. Böttcher, J. O. Delfs, T. Fischer, U. J. Görke, T. Kalbacher, G. Kosakowski, C. I. McDermott, C. H. Park, F. Radu, K. Rink, H. Shao, H. B. Shao, F. Sun, Y. Y. Sun, a. K. Singh, J. Taron, M. Walther, W. Wang, N. Watanabe, Y. Wu, M. Xie, W. Xu, and B. Zehner. OpenGeoSys: an open-source initiative for numerical simulation of thermo-hydro-mechanical/chemical (THM/C) processes in porous media. *Environmental Earth Sciences*, 67(2):589–599, 2012. ISSN 1866-6280. doi: 10.1007/s12665-012-1546-x.
- Olaf Kolditz. *Computational methods in environmental fluid mechanics*. Springer, 2002. ISBN 3-540-42895-x.

-
- Hideo Komine. Predicting hydraulic conductivity of sandbentonite mixture backfill before and after swelling deformation for underground disposal of radioactive wastes. *Engineering Geology*, 114(3-4):123–134, 2010. ISSN 00137952. doi: 10.1016/j.enggeo.2010.04.009.
- Hideo Komine and Nobuhide Ogata. Prediction for swelling characteristics of compacted bentonite. *Canadian Geotechnical Journal*, 33:11–22, 1996.
- Hideo Komine and Nobuhide Ogata. New equations for swelling characteristics of bentonite based buffer materials. *Canadian Geotechnical Journal*, 2003.
- Klaus-Peter Kröhn. New conceptual models for the resaturation of bentonite. *Applied Clay Science*, 23(1-4):25–33, 2003. ISSN 01691317. doi: 10.1016/S0169-1317(03)00083-8.
- David A Laird. Influence of layer charge on swelling of smectites. *Applied Clay Science*, 34: 74–87, 2006. doi: 10.1016/j.clay.2006.01.009.
- David A. Laird, C. Shang, and M.L. Thompson. Hysteresis in crystalline swelling of smectites. *Journal of colloid and interface science*, 171:240–245, 1995.
- Lyesse Laloui and Mathieu Nuth. An introduction to the constitutive modelling of unsaturated soils. *Revue Européenne de Génie Civil*, 9(5-6):651–669, 2005. ISSN 1774-7120. doi: 10.1080/17747120.2005.9692775.
- R W Lewis and B A Schrefler. *The finite element method in the static and dynamic deformation and consolidation of porous media*. John Wiley & Sons Ltd, 1998.
- Guojun Liao and Jiaying Xue. Moving meshes by the deformation method. *Journal of Computational and Applied Mathematics*, 195(1-2):83–92, 2006. ISSN 03770427. doi: 10.1016/j.cam.2005.07.022.
- William J. Likos and Ning Lu. Pore-scale analysis of bulk volume change from crystalline interlayer swelling in Na^+ and Ca^{2+} smectite. *Clays and Clay Minerals*, 54(4):516–529, 2006. ISSN 00098604. doi: 10.1346/CCMN.2006.0540412.
- Longcheng Liu. Permeability and expansibility of sodium bentonite in dilute solutions. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, 358(1-3):68–78, 2010. ISSN 09277757. doi: 10.1016/j.colsurfa.2010.01.033.
- Longcheng Liu, Luis Moreno, and Ivars Neretnieks. A dynamic force balance model for colloidal expansion and its DLVO-based application. *Langmuir*, 25(2):679–687, 2009. ISSN 07437463. doi: 10.1021/la8026573.
- Longcheng Liu, Ivars Neretnieks, and Luis Moreno. Permeability and expansibility of natural bentonite MX-80 in distilled water. *Physics and Chemistry of the Earth, Parts A/B/C*, 36(17-18): 1783–1791, 2011. ISSN 14747065. doi: 10.1016/j.pce.2011.07.009.
- A. Lloret and E. E. Alonso. State Surfaces for partially saturated soils. In *Proceedings of the International Conference on Soil Mechanics and Foundation Engineering*, pages 557–562. AA Balkema, 1985.
- A. Lloret, M. V. Villar, E. E. Alonso, M. Sánchez, A. Gens, and X. Pintado. Mechanical behaviour of heavily compacted bentonite under high suction changes. *Géotechnique*, 53(1): 27–40, 2003. ISSN 0016-8505. doi: 10.1680/geot.2003.53.1.27.

-
- Philip F Low. The Swelling of Clay: II. Montmorillonites. *Soil Science Society of America Journal*, 44(7832):667–676, 1980.
- Philip F. Low. Structural component of the swelling pressure of clays. *Langmuir*, 3(1):18–25, 1987. ISSN 0743-7463. doi: 10.1021/la00073a004.
- G. Lowenthal and P. Airey. *Practical applications of radioactivity and nuclear radiations*. Cambridge University Press, 2001.
- D. M. C. MacEwan and M. J. Wilson. Interlayer and Intercalation Complexes of Clay Minerals. In *Mineralogical Society Monograph No. 5: Crystal Structures of Clay Minerals and their X-Ray Identification*, pages 197–248. Mineralogical Society, 1980.
- Fritz T Madsen and Max Müller-Vonmoos. The swelling behaviour of clays. *Applied Clay Science*, 4(2):143–156, 1989. ISSN 01691317. doi: 10.1016/0169-1317(89)90005-7.
- Duilio Marcial, Pierre Delage, and Yu Jun Cui. On the high stress compression of bentonites. *Canadian Geotechnical Journal*, 39:812–820, 2002. doi: 10.1139/T02-019.
- E.L. Matyas and H.S. Radhakrishna. Volume Change Characteristics of Partially Saturated Soils. *Géotechnique*, 4(18):432–448, 1968.
- J.C. Mayor, M.V. Villar, P.L. Martin, A. Gens, and M. Velasco. Water Uptake in the Bentonite Buffer. In A Schäfers and S Fahland, editors, *International Conference on the Performance of Engineered Barriers (PEBS). Physical and Chemical Properties, Behaviour & Evolution*, pages 15–22, 2014.
- NAGRA. The NAGRA Research, Development and Demonstration (RD&D) Plan for the Disposal of Radioactive Waste in Switzerland. Technical Report TR-09-06, 2009.
- Vicente Navarro, Laura Asensio, Ángel Yustres, Xavier Pintado, and Juan Alonso. An elastoplastic model of bentonite free swelling. *Engineering Geology*, 181:190–201, 2014. ISSN 00137952. doi: 10.1016/j.enggeo.2014.07.014.
- Vicente Navarro, Laura Asensio, Gema De la Morena, Xavier Pintado, and Ángel Yustres. Differentiated intra- and inter-aggregate water content models of MX-80 bentonite. *Applied Clay Science*, 2015. ISSN 01691317. doi: 10.1016/j.clay.2015.10.015.
- NDA. Radioactive Materials Not Reported in the 2010 UK Radioactive Waste Inventory 1. Technical report, 2010.
- NDA. Geological disposal: Overview of international siting processes. Technical report, 2013.
- T.S. Nguyen, G. Armand, and A.P.S. Selvadurai. Modelling the FEBEX THM experiment using a state surface approach. *International Journal of Rock Mechanics and Mining Sciences*, 42(5-6): 639–651, 2005. ISSN 13651609. doi: 10.1016/j.ijrmms.2005.03.005.
- NIREX. Nirex report n/041: Radioactive wastes in the uk: A summary of the 2001 inventory. Technical report, 2002.
- K. Norrish. The swelling of montmorillonite. *Discussions of the Faraday Society*, pages 120–134, 1954.

-
- Mathieu Nuth and Lyesse Laloui. Effective stress concept in unsaturated soils: clarification and validation of a unified framework. *International Journal for numerical and analytical methods in geomechanics*, 32:771–801, 2008. doi: 10.1002/nag.
- S. Olejnik, A. M. Posner, and J. P. Quirk. SWELLING OF MONTMORILLONITE IN POLAR ORGANIC LIQUIDS. *Clays and Clay Minerals*, 22:361–365, 1974.
- B. Palacios, J.L. García-Siñeriz, and J.C. Mayor. Outcome of the Dismantling of “EB” Experiment. In A. Schäfers and S. Fahland, editors, *International Conference on the Performance of Engineered Barriers (PEBS). Physical and Chemical Properties, Behaviour & Evolution*, pages 45–52, 2014.
- H.Q. Pham. *A volume-mass constitutive model for unsaturated soils*. PhD thesis, University of Saskatchewan, 2005.
- Hung Q. Pham and Delwyn G. Fredlund. Volumemass unsaturated soil constitutive model for drying-wetting under isotropic loading-unloading conditions. *Canadian Geotechnical Journal*, 48(2):280–313, 2011. ISSN 0008-3674. doi: 10.1139/t10-061.
- POSIVA. Interim Summary Report of the Safety Case Interim Summary Report of the Safety Case. Technical Report March, 2010.
- R Pusch and R Yong. Water saturation and retention of hydrophilic clay buffer-microstructural aspects. *Applied Clay Science*, 23(1-4):61–68, 2003. ISSN 01691317. doi: 10.1016/S0169-1317(03)00087-5.
- Roland Pusch. Microstructural evolution of buffers. *Engineering Geology*, 54(1-2):33–41, 1999. ISSN 00137952. doi: 10.1016/S0013-7952(99)00059-9.
- Roland Pusch and RN Raymond N Yong. *Microstructure of Smectite Clays and Engineering Performance*, volume 5. Taylor & Francis, 2006. ISBN 0415368634. doi: 10.1016/S1474-4422(06)70500-2.
- Roland Pusch, Ola Karnland, and Harald Hökmark. GMM - A general microstructural model for qualitative and quantitative studies of smectite clays. Technical Report TR-90-43, SKB, 1990.
- Klaus Rathfelder and Linda M. Abriola. Mass conservative numerical solutions of the head-based Richards equation. *Water Resources Research*, 30(9):2579, 1994. ISSN 0043-1397. doi: 10.1029/94WR01302.
- E. Romero, A. Gens, and A. Lloret. Suction effects on a compacted clay under non-isothermal conditions. *Géotechnique*, 53(1):65–81, 2003. ISSN 0016-8505. doi: 10.1680/geot.53.1.65.37254.
- J. Rutqvist, D. Barr, R. Datta, A. Gens, A. Millard, S. Olivella, C.-F. Tsang, and Y. Tsang. Coupled thermal-hydrological-mechanical analyses of the Yucca Mountain Drift Scale Test-Comparison of field measurements to predictions of four different numerical models. *International Journal of Rock Mechanics and Mining Sciences*, 42(5-6):680–697, 2005. ISSN 13651609. doi: 10.1016/j.ijrmms.2005.03.008.

-
- Jonny Rutqvist, Yuji Ijiri, and Hajime Yamamoto. Implementation of the Barcelona Basic Model into TOUGH-FLAC for simulations of the geomechanical behavior of unsaturated soils. *Computers & Geosciences*, 37(6):751–762, 2011. ISSN 00983004. doi: 10.1016/j.cageo.2010.10.011.
- Simona Saba. *Hydro-mechanical behaviour of bentonite-sand mixture used as sealing materials in radioactive waste disposal galleries*. PhD thesis, Université Paris-Est, 2014.
- Simona Saba, Jean-Dominique Barnichon, Yu-Jun Cui, Anh Minh Tang, and Pierre Delage. Microstructure and anisotropic swelling behaviour of compacted bentonite/sand mixture. *Journal of Rock Mechanics and Geotechnical Engineering*, 6(2):126–132, 2014. ISSN 16747755. doi: 10.1016/j.jrmge.2014.01.006.
- Marcelo Sánchez, Antonio Gens, Leonardo do Nascimento Guimarães, and Sebastián Olivella. A double structure generalized plasticity model for expansive materials. *International Journal for Numerical and Analytical Methods in Geomechanics*, 29(8):751–787, 2005. ISSN 0363-9061. doi: 10.1002/nag.434.
- Haruo Sato. Thermodynamic model on swelling of bentonite buffer and backfill materials. *Physics and Chemistry of the Earth, Parts A/B/C*, 33:S538–S543, 2008. ISSN 14747065. doi: 10.1016/j.pce.2008.10.022.
- Tsutomu Sato, Takashi Watanabe, and Ryohei Otsuka. EFFECTS OF LAYER CHARGE , CHARGE LOCATION , AND ENERGY CHANGE ON EXPANSION PROPERTIES OF DIOCTAHEDRAL SMECTITES. *Clays and Clay Minerals*, 40(1):103–113, 1992.
- Tom Schanz and Snehasis Tripathy. Swelling pressure of a divalent-rich bentonite: Diffuse double-layer theory revisited. *Water Resources Research*, 45, 2009. ISSN 0043-1397.
- A.N. Schofield and C.P. Wroth. Critical State Soil Mechanics. *Soil Use and Management*, 25(3): 310, 1968. doi: 10.1111/j.1475-2743.1987.tb00718.x.
- P. Sellin, J.L. García-Siñeriz, A. Dueck, J.C. Mayor, M.V. Villar, P.L. Martin, A. Gens, O. Kristensson, E.E. Alonso, and I. Gaus. HM Evolution of the BUffer. In A. Schäfers and S. Fahland, editors, *International Conference on the Perforance of Engineered Barriers (PEBS). Physical and Chemical Properties, Behaviour & Evolution*, pages 29–34, 2014.
- Daichao Sheng, Delwyn G. Fredlund, and Antonio Gens. A new modelling approach for unsaturated soils using independent stress variables. *Canadian Geotechnical Journal*, 45(4): 511–534, 2008. ISSN 0008-3674. doi: 10.1139/T07-112.
- A. Singh, PLloret and Wesley W. Wallender. Effects of Adsorbed Water Layer in Predicting Saturated Hydraulic Conductivity for Clays with Kozeny Carman Equation. *Journal of geotechnical and environmental engineering*, 134:829–836, 2008. ISSN 1090-0241. doi: 10.1061/(ASCE)1090-0241(2008)134:6(829).
- K. Stein, T. Tezduyar, and R. Benney. Mesh Moving Techniques for Fluid-Structure Interactions With Large Displacements. *Journal of Applied Mechanics*, 70(1):58, 2003. ISSN 00218936. doi: 10.1115/1.1530635.

-
- A. M. Tang and Y. J. Cui. Effects of mineralogy on thermo-hydro-mechanical parameters of MX80 bentonite. *Journal of Rock Mechanics and Geotechnical Engineering*, 2(1):91–96, 2010. doi: 10.3724/SPJ.1235.2010.00091.
- Hywel Rhys Thomas, Peter John Cleall, N Chandler, D Dixon, and H P Mitchell. Water infiltration into a large-scale in-situ experiment in an underground research laboratory. *Géotechnique*, 53(2):207–224, 2003. ISSN 0016-8505. doi: 10.1680/geot.2003.53.2.207.
- Carsten Thorenz. *Model Adaptive Simulation of Multiphase and Density Driven Flow in Fractured and Porous Media*. PhD thesis, 2001.
- Snehasis Tripathy, Asuri Sridharan, and Tom Schanz. Swelling pressures of compacted bentonites from diffuse double layer theory. *Canadian Geotechnical Journal*, 41:437–450, 2004. doi: 10.1139/T03-096.
- Chin-Fu Tsang. Introductory editorial to the special issue on the DECOVALEX-THMC project. *Environmental Geology*, 57(6):1217–1219, 2008. ISSN 0943-0105. doi: 10.1007/s00254-008-1626-0.
- A. Tsiamposi, L. Zdravkovic, and D.M Potts. A three-dimensional hysteretic soil-water retention curve. *Geotechnique*, 65(2):155–164, 2013.
- C. Tweed, A. Ellis, and R. Whittlestone. Delivering safe geological disposal of nuclear waste in the UK. In *Proceedings of the Institution of Civil Engineers*, volume 168. ICE Publishing, 2015.
- M. Th. van Genuchten. A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. *Soil Science Society of America Journal*, 44:892–898, 1980.
- H. van Olphen. Thermodynamics of interlayer adsorption of water in clays I-Sodium Vermiculite. *Journal of Colloid Science*, 7(394), 1965.
- M.V. V Villar, R. Gómez-Espina, and L. Gutiérrez-Nebot. Basal spacings of smectite in compacted bentonite. *Applied Clay Science*, 65-66:95–105, 2012. ISSN 01691317. doi: 10.1016/j.clay.2012.05.010.
- Qiong Wang. *Hydro-mechanical behaviour of bentonite-based materials used for high-level radioactive waste disposal*. PhD thesis, 2012.
- Qiong Wang, Anh Minh Tang, Yu-Jun Cui, Pierre Delage, and Behrouz Gatmiri. Experimental study on the swelling behaviour of bentonite/claystone mixture. *Engineering Geology*, 124: 59–66, 2012. ISSN 00137952. doi: 10.1016/j.enggeo.2011.10.003.
- Qiong Wang, Yu-Jun Cui, Anh Minh Tang, Li Xiang-Ling, and Ye Wei-Min. Time- and density-dependent microstructure features of compacted bentonite. *Soils and Foundations*, 54(4):657–666, 2014. ISSN 00380806. doi: 10.1016/j.sandf.2014.06.021.
- A. Wayllace. *VOLUME CHANGE AND SWELLING PRESSURE OF EXPANSIVE CLAY IN THE CRYSTALLINE SWELLING REGIME*. PhD thesis, 2008.
- Zhijian Wen. Selection and Basic Properties of the Buffer Material for High-Level Radioactive Waste Repository in China 3 Historical Practices of Buffer Study in China 4 Bentonite Deposits in China. *ACTA GEOLOGICA SINICA*, 82(5):1050–1055, 2008.

-
- S. J. Wheeler and V. Sivakumar. An elasto-plastic critical state framework for unsaturated soil. *Géotechnique*, 45(1):35–53, 1995. ISSN 0016-8505. doi: 10.1680/geot.1995.45.1.35.
- www.ceaa-acee.gc.ca. <http://www.ceaa-acee.gc.ca/050/document-eng.cfm?document=103943>. Accessed: 05/02/2016.
- www.igdtp.eu. www.igdtp.eu. Accessed: 01/12/15.
- www.nda.gov.uk. www.nda.gov.uk/2015/11/world-first-for-finland/. Accessed: 28/11/2015.
- www.opengeosys.org. www.opengeosys.org. Accessed: 12/11/2013.
- W.M. M Ye, Y.J. J Cui, L.X. X Qian, and B. Chen. An experimental study of the water transfer through confined compacted GMZ bentonite. *Engineering Geology*, 108(3-4):169–176, oct 2009. ISSN 00137952. doi: 10.1016/j.enggeo.2009.08.003.
- R.N. Yong. Soil suction and soil-water potentials in swelling clays in engineered clay barriers. *Engineering Geology*, 54(1-2):3–13, 1999a. ISSN 00137952. doi: 10.1016/S0013-7952(99)00056-3.
- R.N. Yong. Overview of modeling of clay microstructure and interactions for prediction of waste isolation barrier performance. *Engineering Geology*, 54(1-2):83–91, 1999b. ISSN 00137952. doi: 10.1016/S0013-7952(99)00064-2.
- Paul A. Zegeling. r-refinement for evolutionary PDEs with finite elements or finite differences. *Applied Numerical Mathematics*, 26(1-2):97–104, 1998. ISSN 01689274. doi: 10.1016/S0168-9274(97)00086-X.
- F. Zhang, Philip F. Low, and Charles B. Roth. Effects of monovalent, exchangeable cations and electrolytes on the relation between swelling pressure and interlayer distance in montmorillonite. *Journal of colloid and interface science*, 173:34–41, 1995.
- Xiong Zhang and R.L. Lytton. *Use of state surface approach to explain the Barcelona Basic Model*, chapter in: Theoretical and Numerical Unsaturated Soil Mechanics. Springer, 2007.
- An-Nan Zhou, Daichao Sheng, Scott W. Sloan, and Antonio Gens. Interpretation of unsaturated soil behaviour in the stress Saturation space, I: Volume change and water retention behaviour. *Computers and Geotechnics*, 43:178–187, jun 2012. ISSN 0266352X. doi: 10.1016/j.compgeo.2012.04.010.

Appendix A

List of implemented and edited functions

This project has involved significant development of the open source objected oriented code OpenGeoSys. Provided with this thesis is a digital appendix that includes the source code and the models. In addition to this, this appendix chapter provides a list of implemented functions along with a short description of their function. In the following, function arguments are omitted to avoid clutter and confusion.

A.1 Class: MeshElement

Get and set functions were defined for the following element variables:

- `ElementVolume`: For use in calculation of strain dependent parameters.
- `VirtualElementVolume`: For use in calculation of strain dependent parameters of the virtual mesh.
- `OriginalElementVolume`: For total strain calculation.
- `IncrementalVStrain`: Determining the direction of strain for the previous time-step.
- `Virtual_IncrementalVStrain`: Determining the direction of strain for the previous time-step in the virtual mesh.
- `VolumetricStrain`: Total volumetric strain for calculation of new Young's Modulus.
- `ElementPorosity`: For use in the calculation of permeability and the building of the mass matrix.
- `ElementVoidRatio`: Used in definition of new Young's modulus.
- `InitialElementVoidRatio`: Used in definition of new Young's modulus.
- `ElementYoungsModulus`: Variable dependent on the volumetric strain.
- `ElementDryDensity`: For use in the calculation of element saturation.
- `ElementMassSolids`: For calculation of dry density.

A.2 Class: CElement

- `interpolate_point()`: As described in Chapter 4, this function interpolates the mesh node values to the global point coordinates.
- `ConfigVirtualElement()`: Configures the element in the virtual mesh
- `ConfigElement()`: This existing function was edited for use with the moving mesh application

A.3 Class: CFiniteElementStd

- `CalCoefMass()`: The Richards equation implementation has been edited to calculate the current porosity, dry density, and maximum water content in the virtual element.
- `CalCoefLaplace()`: The Richards equation implementation has been edited to calculate the current porosity, dry density, and maximum water content in the virtual element.
- `UpdateRichards()`: This function calculates the free swell suction from the calculated net suction and the confining stress. Essentially, this calculates total suction for the next time-step.
- `ResetRichards()`: This calculates the net suction at the beginning of the time-step as a function of the confining stress and total suction.
- `CalcAxisymVol()`: Calculates the moving mesh element volume in an axisymmetric mesh.
- `CalcSaturation()`: This function has been edited to include the water content variable along with saturation.
- `CalcAxisymVirtualVol_end()`: Calculate the virtual element volume in an axisymmetric model at the end of a time-step.
- `CalcNodeMatParameter()`: This has been extended to include the calculation and interpolation of element properties of dry density, porosity, and Young's Modulus.

A.4 Class: CFiniteElementVec

- `LocalAssembly_continuum()`: Multiple edits for use with the non-linear elastic model, including the coupling mechanism of the hydraulics to the mechanics via the internal strain factor.
- `ExtrapolateGaussStrainDM()`: Extrapolation of strain at gauss points to nodes in a moving mesh non-linear elastic application.

A.5 Class: COutput

- `NODWritePLYDataTEC()`: Edited to include the moving mesh coordinates.
- `NODWritePNTDataTEC()`: Edited to include flexibility for a moving point or a fixed interpolated point.

A.6 Class: CRFProcessDeformation

- `InitialiseVirtualMesh()`: Sets the original virtual mesh coordinates to the same as the global mesh.
- `UpdateIterativeStep()`: This has been edited to prevent the calculated displacement being added to the new location of the moving mesh.

A.7 Class: CRFProcess

- `GetInterpolatedPointValue()`: Calls `interpolate_point` to return the value at the global point coordinate.
- `IncorporateBoundaryConditions()`: This function has been extended to include the displacement dependent boundary conditions for both the axisymmetric and 2D plane strain models.
- `IncorporateSourceTerms()`: This function has been edited to include a switch for the application of the source term in the NLE-ST model.
- `VirtualMesh()`: Created to update the virtual mesh nodal coordinates with the displacement calculated at the end of the DEFORMATION process.
- `UpdateRichardsPc()`: Calls `UpdateRichards()` to set the free-swell suction after a time-step has been accepted.
- `ResetRichardsPC()`: This function calls `ResetRichards()` at the start of the hydraulic process i.e. within each iteration of the hydraulic and mechanic processes. This allows the mechanical stress conditions change of confinement loss to be transferred to the hydraulic process.
- `Extrapolation.Secondary_Variables.Vol()`: Calls `UpdateSecondaryVariablesMeshCoordinates()` and calculates the element volume at the end of the time-step.
- `Extrapolation.Secondary_Variables.DM()`: Calls the calculation of volumetric strain, void ratio, and dry density. Also sets the switch for the source term in `IncorporateSourceTerms()`.
- `UpdateVirtualMeshCoordinates()`: Adds the calculated displacement to the virtual mesh nodal coordinates and sets the new locations in the virtual mesh.
- `SetOriginalMeshCoordinates()`: Sets the coordinates of the nodes at initial conditions for comparison of deformation.

- `CalcSecondaryVariablesUpdateMeshCoordinates()`: Adds the calculated displacement to the global mesh nodes and set the new nodal locations.
- `CalcSecondaryVariablesVolumetricStrain()`: Calculates the volumetric strain of each element.
- `CalcSecondaryVariablesVirtualVolumetricStrain()`: Calculates the volumetric strain of the virtual element.
- `CalcSecondaryVariablesVoidRatio()`: Calculates a new element void ratio from the new element volume at the end of the time-step.
- `CalcSecondaryVariablesVoidRatio()`: Calculates a new virtual element void ratio from the new virtual element volume.
- `CalcSecondaryVariablesDryDensity()`: Calculates a new element dry density from the new element volume.
- `CalcSecondaryVirtualVariablesDryDensity()`: Calculates a new virtual element dry density from the new virtual element volume.
- `CalcSecondaryVariablesSwellPressure()`: Calculates the net mean stress at every node in the model. It also integrates the axial stress across the top boundary in an axisymmetric model.

A.8 Class: Problem

- `CouplingLoop()`: This was edited to include the error control on the coupling between the hydraulic and mechanical processes.
- `PreLoop()`: This was edited to call `ResetRichardsPC()`.

A.9 Class: CBoundaryCondition

A number of Get and Set functions were implemented for use with the displacement dependent boundary conditions:

- `getDispLimit()`
- `getDisp_Direction()`

A.10 Class: CMediumProperties

- `Porosity`: An updating porosity model based on the element volume.
- `PermeabilityTensor()`: A number of permeability models were implemented.
- `SaturationCapillaryPressureFunction()`: A new case for the implementation of the stress dependent water retention behaviour (Dueck suction) was created.

- `SaturationCapillaryPressureFunction_wc_S()`: This was created to perform the calculation of the previous function, but to calculate the saturation as opposed to the water content.
- `Rho_d()`: Calculation of the dry density at each element.
- `PermeabilitySaturationFuction()`: A power law relative permeability was implemented in this function.

A.11 Class: `CSolidProperties`

- `variableInternal_Strain_Factor()`: Functions for the dependency of the internal strain factor on water content, or saturation.
- `Youngs_Modulus()`: A new case for the calculation of the non-linear elastic function was created.

A.12 `tools.cpp`

- `GetCurveDerivative_wc_S()`: This function calculates the derivative of saturation with respect to suction pressure from the relationship between water content and suction pressure, as discussed in Chapter 4.

A.13 Class: `CFEMesh`

- `GetNearestElement()`: Calls `calcSumAreas_Tri()` to determine the element within which a fixed geometric point is in a moving mesh. For use with the Interpolated point output function.