An Investigation of the Thermo/Hydro/Mechanical Behaviour of Large Scale Experiments

- including Parametric Studies on Various Critical Factors

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Declaration

This work has not previously been accepted in substance for any degree and is not concurrently submitted in candidature for any degree.

Signed ...........................................(Chun Yean Tey)
Date 31/12/2004

Statement 1

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"Our greatest glory is not in never falling, but in rising every time we fall"

Confucius (551 BC – 479 BC)
Summary

This thesis presents an investigation into the thermo/hydro/mechanical interactions occurring in two large scale experiments with different geometry setup designed for deep geological disposal of nuclear waste.

The analysis of flow and deformation through unsaturated soils was performed using the proposed constitutive model. The following mechanisms are accommodated; moisture flow in liquid and vapour forms, dry air flow including the movement of bulk air and the transport of dissolved air in the pore water, heat transfer by conduction, convection and latent heat of vapourisation, and the elasto-plastic deformation of unsaturated soils. The governing differential equations are solved spatially using a finite element technique and temporally using a finite difference technique.

The numerical model was subsequently applied to two large scale experiments: AECL’s Buffer/ Container Experiment and AECL’s Horizontal Canister In-room geometry. The analyses involved modelling the coupled thermo/hydro/mechanical interaction between the engineered buffer and the host rock, and the swelling phenomena at the buffer/rock interface. A comprehensive set of material parameters was determined for use in the numerical code.

A theoretical formulation was developed to describe a time-dependent adsorption/desorption process associated with the micro/macro swelling phenomena occurring in bentonite-based buffer materials. This was implemented within the numerical model. The transient swelling behaviour of bentonite-based buffer materials was found to be influential in the simulation of an underground repository, in particular the resaturation behaviour in expansive clay.

Sensitivity analyses on critical parameters identified for both geometry setups are presented and shown to affect the resaturation processes to varying degrees. This investigation has provided valuable insights into the repositories’ behaviour.
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Notation

\(a\) Constant
\(A_t\) Defined in equation (3.116)
\(A_r\) Defined in equation (3.116)
\(A\) Defined in equation (3.132)
\(b\) Constant
\(b_x, b_y\) Two-dimensional body forces
\(B\) Defined in equation (3.38)
\(b\) Body force vector
\(B\) Strain-displacement matrix
\(c\) Constant
\(C_{ao}\) Defined in equation (3.71)
\(C_{at}\) Defined in equation (3.69)
\(C_{atT}\) Defined in equation (3.70)
\(C_{an}\) Defined in equation (3.72)
\(C_{iI}\) Defined in equation (3.50)
\(C_{iT}\) Defined in equation (3.51)
\(C_{iu}\) Defined in equation (3.53)
\(C_{p,ao}\) Specific heat capacity of dry air
\(C_{p,li}\) Specific heat capacity of liquid
\(C_{p,s}\) Specific heat capacity of soil solids
\(C_{p,v}\) Specific heat capacity of vapour
\(C_{Tt}\) Defined in equation (3.94)
\(C_{TtT}\) Defined in equation (3.95)
\(C_{Tu}\) Defined in equation (3.97)
\(C_{oo}\) Defined in equation (3.139)
\(C_{ot}\) Defined in equation (3.137)
\(C_{oiT}\) Defined in equation (3.138)
\(C_{ou}\) Defined in equation (3.140)
\(C\) Defined in equation (4.60)
C_{aa} Defined in equation (4.35)
C_{ai} Defined in equation (4.33)
C_{aT} Defined in equation (4.34)
C_{an} Defined in equation (4.36)
C_{a} Defined in equation (4.15)
C_{IT} Defined in equation (4.16)
C_{ia} Defined in equation (4.18)
C_{Ta} Defined in equation (4.26)
C_{Tn} Defined in equation (4.24)
C_{TT} Defined in equation (4.25)
C_{Tn} Defined in equation (4.27)

D_{om} Molecular diffusivity of vapour through air
D_{d} Coefficient of molecular diffusion.
D_{h} Coefficient of hydrodynamic dispersion
D_{m} Coefficient of mechanical dispersion
D_{T} Temperature effect factor on vapour velocity
D_{Mv} Suction effect factor on vapour velocity
D Elasticity matrix
\hat{D} Revised elasticity matrix
\tilde{D} Revised elasticity matrix
e Void ratio
e_0 Initial void ratio
E Young's modulus
E_{ss} Source or sink term
f Flow area factor
F_x, F_y Resultant forces in x, y directions
f_a Defined in equation (4.39)
f_i Defined in equation (4.22)
f_T Defined in equation (4.31)
g Gravitational constant
Defined in equation (3.39)

Shear modulus

Specific weight

Relative humidity

Heat capacity of the soil

Henry's volumetric coefficient of solubility

Unit matrix

Defined in equation (3.75)

Defined in equation (3.57)

Defined in equation (3.102)

Effective permeability of pore-liquid

Effective permeability of pore-air

hydraulic conductivity for swelling clay

Bulk modulus

Coefficient of earth pressure at rest

Unsaturated conductivity of air

Defined in equation (3.74)

Defined in equation (3.73)

Unsaturated hydraulic conductivity

Defined in equation (3.56)

Defined in equation (3.54)

Defined in equation (3.55)

Defined in equation (3.101)

Defined in equation (3.99)

Defined in equation (3.100)

Defined in equation (4.38)

Defined in equation (4.37)

Defined in equation (4.21)

Defined in equation (4.19)

Defined in equation (4.20)

Defined in equation (4.30)
$K_{\tau\tau}$ Defined in equation (4.28)
$K_{RT}$ Defined in equation (4.29)
$L$ Latent heat of vapourisation
$M$ Slope of the critical state line
$M_f$ Curving fitting factor
$m$ Unit vector
$n$ Porosity
$N_A$ Avagadro’s constant
$N_r, N_s$ Shape functions
$N(s)$ Intercept of the normal compression line for a soil at suction $s$
$N(0)$ Intercept of the normal compression line for the saturated soil
$N$ Matrix of shape functions
$p$ Net mean stress
$p_{atm}$ Atmospheric pressure
$p_i$ Initial net mean stress
$p_c$ Reference stress
$p_s$ Parameter controlling suction effect on cohesion
$p_0$ Preconsolidation stress at a suction $s$
$p_0^*$ Saturated preconsolidation stress
$q$ deviatoric stress
$Q$ Heat flux per unit area
$Q_1$ Plastic potential for LC yield surface
$Q_2$ Plastic potential for SI yield surface
$Q_3$ Plastic potential for SI$_m$ yield surface
$Q_4$ Plastic potential for SD$_m$ yield surface
$r$ Constant related to the maximum stiffness of the soil
$R_{\Omega}$ Residual error introduced due to approximation
$R_{da}$ Specific gas constant for dry air
$R_v$ Specific gas constant for water vapour
$s$ Suction at a temperature $T$
$s_i$ Initial suction
$s_r$ Suction at reference temperature
$s_0$ Critical value of suction - suction hardening parameter
$S$ Specific surface
$S_a$ Degree of saturation of pore-air
$S_l$ Degree of saturation of pore-liquid
$S_{ro}$ Initial degree of saturation of pore-liquid
$S_{free}$ Degree of saturation for free water
$S_{ab}$ Degree of saturation for adsorbed water
$t$ Time
$T$ Temperature
$T_r$ Reference temperature
$\hat{T}$ Approximate value of temperature
$(\nabla T)_a/\nabla T$ Ratio of the microscopic temperature gradient in pore space to the macroscopic temperature gradient
$T_s$ Nodal value of temperature
$\mathbf{TL}_{abs}$ Matrix of absolute tolerances
$\mathbf{TL}_{rel}$ Matrix of percentage tolerances
$u$ Defined in equation (8.3)
$u_a$ Pore-air pressure
$u_{da}$ Partial pressure of dry air
$u_l$ Pore-water pressure
$u_v$ Partial pressure of water vapour in pore space
$\hat{u}_a$ Approximate value of pore-air pressure
$\hat{u}_l$ Approximate value of pore-water pressure
$\hat{u}$ Approximate value of displacement
$u_{var}$ Defined in equation (4.1)
$\mathbf{u}$ Displacement vector
$u_{a,s}$ Nodal value of pore-air pressure
$u_{l,s}$ Nodal value of pore-water pressure
$u_s$ Nodal value of displacement
$v$ specific volume
$v_i$ Initial specific volume
$v_v$ Mass flow factor  
$V_w$ Specific water volume  
$v_a$ Velocity of air  
$v_l$ Velocity of liquid  
$v_{l_i}$ Velocity of liquid due to chemical solute gradients.  
$v_{l_i}$ Velocity of liquid due to pore water pressure and elevation heads  
$v_v$ Velocity of water vapour  
$w$ Water content  
$w_a$ percentage of water that is adsorbed  
$w_f$ percentage of free water  
$w_l$ Liquid limit  
$w_{max}$ Maximum adsorbed water percentage  
$w_0$ Initial water content  
$w_p$ Plastic limit  
$w_n$ Liquidity index  
$x, y, z$ Global coordinates  
$\alpha$ Constant  
$\alpha_q$ Parameter for non-associated flow rule  
$\alpha_T$ Coefficient of thermal expansion  
$\beta$ Parameter controlling the rate of increase of soil stiffness with suction  
$\chi$ Parameter associated with the effective stress relationship of equation  
$\chi_1, \chi_2$ Fluidity parameters controlling the plastic flow rate  
$\varepsilon$ Total strain  
$\varepsilon'$ Elastic component of strain  
$\varepsilon''$ Plastic component of strain  
$\varepsilon'''$ Rate of viscoplastic strain  
$\varepsilon_{*}'$ Elastic component of strain due to effective stress changes in the microstructure
\( \varepsilon_{M_s} \) Elastic component of strain due to suction changes in the macrostructure

\( \varepsilon_{M_D} \) Elastic component of strain due to net stress changes in the macrostructure

\( \varepsilon' \) Elastic deviatoric strain

\( \varepsilon'' \) Plastic deviatoric strain

\( \varepsilon_s \) Static permittivity of medium

\( \varepsilon_s' \) Elastic component of strain due to suction changes

\( \varepsilon_T \) Elastic component of strain due to temperature changes

\( \varepsilon_v \) Volumetric strain

\( \varepsilon'' \) Total volumetric plastic strain

\( \varepsilon''_{\text{rm}} \) Defined in equation (3.236)

\( \varepsilon''_{\text{vp}} \) Volumetric plastic strain due to stress changes

\( \varepsilon''_{(p+s)f} \) Volumetric plastic strain associated with yield surface \( F_3 \)

\( \varepsilon''_{(p+s)f_D} \) Volumetric plastic strain associated with yield surface \( F_4 \)

\( \varepsilon_{s''} \) Volumetric plastic strain due to suction changes

\( \varepsilon''_o \) Elastic component of strain due to stress changes

\( \phi' \) Angle of friction for saturated soils

\( \gamma_l \) Unit weight of liquid

\( \varphi \) Positive increasing function

\( \varphi' \) Angle of friction for saturated soil

\( \kappa \) Stiffness parameter for changes in net mean stress in the elastic region

\( \kappa_s \) Stiffness parameter for changes in suction in the elastic region

\( \lambda_a \) Thermal conductivity of pore-air

\( \lambda_l \) Thermal conductivity of pore-liquid

\( \lambda_s \) Stiffness parameter for changes in suction for virgin states of the soil

\( \lambda_T \) Intrinsic thermal conductivity of soil

\( \lambda_v \) Thermal conductivity of pore-vapour
\( \lambda(0) \) Stiffness parameter for changes in net mean stress for saturated soil
\( \lambda(s) \) Stiffness parameter for changes in net mean stress for virgin states of the soil
\( \mu_a \) Absolute viscosity of air
\( \mu_l \) Absolute viscosity of liquid
\( \theta_a \) Volumetric content of air
\( \theta_l \) Volumetric liquid content of the soil
\( \theta_v \) Volumetric vapour content of the soil
\( \xi \) Surface energy at temperature \( T \)
\( \xi_r \) Surface temperature at reference temperature \( T_r \)
\( \rho_0 \) Saturated soil water vapour
\( \rho_{da} \) Density of dry air
\( \rho_l \) Density of pore-liquid
\( \rho_s \) Density of soil solids
\( \rho_v \) Density of water vapour
\( \sigma \) Total stress (Chapter 2)
\( \sigma' \) Effective stress
\( \sigma'' \) Net total stress
\( \sigma_x, \sigma_y, \sigma_z \) Normal stresses
\( \tau_{xy}, \tau_{xz} \) Shear stresses
\( \tau_v \) Tortousity factor
\( \nu \) Poisson’s ratio
\( \omega \) Required time interval
\( \psi \) Capillary potential
\( \psi_r \) Capillary potential at reference temperature \( T_r \)
\( \Gamma' \) Element boundary surface
\( \delta \) Defined in equation (4.101)
\( \Omega \) Heat content of moist soil
\( \Omega' \) Element domain
\( \phi \) Variable vector
Chapter 1

Introduction

In recent years, the global warming phenomena and greenhouse gas effects have become an issue of major public concern. The rise in carbon dioxide levels arising from the burning of fossil fuels has been identified as the main reason for the greenhouse effects. It is believed that Britain alone produces 560 million tonnes of carbon dioxide. The Kyoto Protocol requires Britain to reduce its carbon dioxide emissions by 12.5% before 2010, which Britain has opted to raise to 20%. Over the years, Britain has attempted to diversify its energy source to other forms of energy. Nuclear power has formed a major component of energy production. In 2000, some 30% of Britain's energy was derived from nuclear power. In other parts of the world, nuclear power has also emerged as a major source of energy. According to the World Nuclear Association (WNA, 2004) there are currently 440 commercial nuclear reactors in 31 countries with over 360,000 MWe of total capacity, catering for 16% of the world's electricity demand.

Although not based on a fossil fuel, there are waste materials from nuclear power generation. It is estimated that each year the United Kingdom produces 20,000m$^3$ of nuclear waste (WNA, 2004). Nuclear waste can be categorised into low level waste, medium level waste, and high level waste. Both low level and medium level waste are relatively easy to dispose of. The level of radioactivity and half life of the radioactive isotopes for these levels of waste are low. High level nuclear waste is the most radioactive and requires thousands of years before it can be deemed safe. As such, the security of the radioactive waste must be assured over geological timescale. It was estimated that in 2002, there was 3500m$^3$ of high level nuclear waste, which accounted for 90% of the total radioactivity of nuclear waste in storage. It is
also estimated that about 250 nuclear facilities from all parts of the world will be waiting to be decommissioned by 2010 (North West, 2004).

A number of options have been considered for high level nuclear waste disposal. Of those that were put forward, most countries believe that deep geological burial presents the best solution for high level nuclear waste disposal. Although the proposed underground disposal layout for various countries may differ, they all serve one common purpose: to act as barrier(s) to the movement of radionuclide. To achieve this, the waste material has to be isolated and remain intact for a long period of time. Both cost effective construction method and reliable technology have to be in place to facilitate such disposal. A key component of the safety assessment of the proposed repositories is the prediction of future performance. To enable the prediction, numerical models capable of simulating radionuclide movement are required, so that researchers can improve the repository design and assess the performance of the barrier system in relation to the radionuclide release.

Typically, there are two types of borehole configuration for the placement of waste canisters: a vertical borehole configuration and a horizontal canister deposition configuration. A typical layout for a vertical borehole configuration is the Canadian concept, illustrated in Figure 1.1. In the proposed repository configuration, the waste canisters would be placed in boreholes drilled in the floor of the underground caverns, backfilled later using a buffer material with the natural host material forming the final barrier. However, a horizontal canister deposition configuration involves placing canisters in horizontal boreholes from access tunnel. A typical layout is illustrated in Figure 1.2. For both sets of configurations, experts will need to ensure the heat generated by waste can be managed by the emplaced system and that no preferential flow network exists. Operability during emplacement of canisters, construction costs and space requirements are some of the key factors when deciding on a suitable borehole configuration.

Atomic Energy of Canada Limited (AECL) has considered both vertical and horizontal placement of waste canisters. The Buffer/Container Experiment, a comprehensive large scale in situ experiment employing a vertical borehole configuration layout had been carried during the mid-1990s. The In-Room Emplacement geometry has been proposed by AECL as a potential design concept.
for a horizontal canister deposition configuration. In the proposed layout, the room is symmetrical with two sets of canisters positioned at mid-height of a tunnel. In both cases, high temperatures would be generated near the canisters, resulting in high temperature gradient between the engineered buffer material and the rock. There would also be moisture migrating away from the buffer material close to the heater and an opposing influx of moisture into the buffer from the saturated host rock. The heating would also produce shrinkage close to the heater and swelling at the interface with the host rock. This work sets out to investigate the thermo/hydro/mechanical behaviour for the Buffer/Container Experiment and the In Room Emplacement geometry, in particular focusing on the resaturation process and its effect on the overall performance.

The coupling processes for the thermal, hydraulic and mechanical responses in a typical geological disposal unit are complex and require highly sophisticated numerical models to simulate these processes. The numerical modelling works carried out in this study have used COMPASS, a finite element modelling code which can model flow and deformation in unsaturated soils. The coupled interactions between the unsaturated engineered buffer material and saturated host rock are investigated. The influence of swelling in microstructure on the overall macro-behaviour is also assessed.

The theoretical model used in this work was initially a potential based fully coupled model for heat, moisture and air transfer developed by Thomas and Sansom (1995). Non-linear elastic and elasto-plastic deformation behaviour have been integrated by Thomas and He (1994, 1995); Thomas and Cleall (1999); and Wang (2000). In this work, the theoretical model which has been incorporated into a numerical model is applied to simulate both the Buffer/Container Experiment and the In Room geometry. At some stages, aspects of the theory have been developed to accommodate phenomena observed in the experiment.

Heat flow due to conduction, convection, and latent heat of vaporisation is governed by a conservation of energy equation. Moisture flow is considered to be a combination of liquid and vapour transfer, and is accounted for by a conservation of mass equation. Moisture movement in both liquid and vapour form, caused by pressure gradients is governed by Darcy’s law, and vapour transfer due to diffusion
is represented by a modified Philip and de Vries approach (1957). The conservation
of mass equation also governs the movement of dry air within the soil. The
movement of dry air may be considered to include both the bulk flow of air and the
movement of dissolved air in the pore liquid. The flow of free air is represented by
Darcy’s Law, whilst Henry’s Law governs the quantity of dissolved air and its flow.
The stress/strain behaviour of the soil is represented with an elasto-plastic
constitutive relationship and is governed by the stress equilibrium equation.

A numerical solution to the theoretical formulation is obtained via spatial
discretisation using the finite element method and temporal discretisation using the
finite difference method. The numerical model is then applied to the
Buffer/Container Experiment and a proposed layout for the In Room Emplacement.
The experimental and numerical results for the Buffer/Container Experiment are
presented and analysed. The simulation performed on the Buffer/Container
Experiment found that a hydraulic conductivity relationship based on the water
exchange between the microstructure and macrostructure in swelling clays, gave
good correlation with the experimental results. The transient water exchange model
is extended to the proposed geometry layout for the In Room Emplacement. The
numerical results are also presented and discussed.

1.1 Study Objectives

The main objectives of this study may be summarised as follows;

- To review the developments made in the modelling of high level nuclear
  waste repositories and investigate the influence of the micro-macro structure
  of clay on moisture flow in a repository set up.

- To develop and implement conceptual models capable of describing the
  effects of swelling phenomena and the effects water at microstructure level
  have on the behaviour of a large scale in situ experiment.

- To investigate the thermo/hydro/mechanical interaction between an
  unsaturated buffer material and a saturated rock, under the effects of thermal
  and hydraulic potential gradients.
• To predict the thermal, hydraulic and mechanical response for the proposed In Room Emplacement geometry setup, using the conceptual model developed for the Buffer/Container Experiment.

• To investigate the influence of some material parameters on the simulated experiments using numerical analysis and improve the understanding of soil interactions between rock and clay barrier.

1.2 Research Background

This section presents a brief review of the research work that has been carried out at Cardiff University and on which this present work is based. In Chapter 2, a wider research review is presented.

A theoretical model of coupled transient heat and moisture transfer in unsaturated soil, including gravity effects was developed by Thomas (1985). Vapour flow was modelled by incorporating the de Vries approach (1958), and the latent heat of vaporisation was based on work by Luikov (1966). Non-linearity of material parameters were later incorporated, (Thomas, 1987; Thomas, 1988a; Thomas, 1988b), and revised time stepping schemes were also investigated (Thomas and Rees, 1988; Thomas and Rees, 1990).

Following an experimental investigation into the behaviour of unsaturated sand surrounding a heating rod (Ewen and Thomas, 1987), Ewen and Thomas (1989) modified the vapour transfer diffusivities of the numerical model to simulate coupled heat and moisture transfer processes in unsaturated soil. Thomas and King (1991) further developed the approach, replacing the primary variable of moisture content with one of capillary potential. In doing so, the theoretical model became compatible with the current approach in unsaturated soil mechanics. The numerical model was then used to simulate the same experiment performed by Ewen and Thomas (1987), and achieved a good correlation. The updated model was then extended to include the effect of elevated pore air pressure, which was presented by Thomas and Sansom (1995). The model was verified by comparison against the results from a number of experiments on sand and clay.
Deformation behaviour was first introduced into the theoretical formulation and later on in a numerical model by Thomas and Rees (1990). Thomas et al., (1992) presented an isothermal coupled model capable of predicting moisture transfer and deformation in unsaturated soils. The deformation behaviour of the soil was represented by the non-linear elastic state surface approach presented by Lloret and Alonso, (1985).

Thomas and He, (1994) further integrated an elasto-plastic constitutive relationship (Alonso et al., 1990) to arrive at a coupled thermo/hydro/mechanical model to investigate the performance of high level nuclear waste disposal schemes. Thomas and Cleall (1999) extended the thermo/hydro/mechanical model to include highly expansive behaviour in soil. Chemical solute and contaminant transport capabilities were also presented in Thomas and Cleall (1997), and developed further to incorporate geochemical reaction by Hashm (1999) and Seetharam (2003).

1.3 Scope and Limitations.

This section details the scope and limitations of the theoretical and numerical formulations used in this study. As described earlier, the theoretical formulation allows for coupled thermo/hydro/mechanical analysis of unsaturated soils. However, it should be noted that the model assumes the soil as homogeneous. Understandably, soils exhibit some heterogeneity and this may be partly accommodated as the assumption of homogeneity only applies within an individual element. Therefore, different soil types may be chosen in a simulation.

The theoretical formulation has been presented in a two dimensional form, which may represent plane strain, plain stress or axisymmetric analysis. However, the numerical code, COMPASS is capable of three dimensional simulations.

The hysterisis effects observed in the water retention curve have not been accounted for in this study.

As for simulating the deformation behaviour in unsaturated soils, the constitutive model implemented for stress/strain behaviour is valid for slightly and moderately expansive soils.
To solve the theoretical governing equations, some form of approximation methods is required. The finite element method is used for spatial discretisation, and a finite difference method is used for temporal discretisation.

1.4 Thesis Overview

A brief description of the contents for each chapter is presented as follows.

Chapter 2 shows a review of developments made in the modelling work on coupled heat, moisture and air transfer, as well as deformation behaviour in unsaturated soil. A review on the influence of microstructure of clay on moisture flow is also presented. Large scale experimental research work aimed at improving the understanding on underground waste disposal is also presented.

Chapter 3 shows the development of a coupled thermo/hydro/mechanical theoretical formulation for an unsaturated soil. Four separate governing equations describing heat, moisture, air flow and deformation are derived and presented.

Chapter 4 presents a numerical solution to the governing equations presented earlier in Chapter 3. Finite element method is applied to achieve spatial discretisation. Finite difference method is used to achieve temporal discretisation.

Chapter 5 presents the identification and characterisation of the material parameters required to simulate AECL's Buffer/Container Experiment and AECL's proposed geometry layout for the In Room Emplacement. The thermal, hydraulic and mechanical material parameters are defined for each of these materials.

Chapter 6 begins by reviewing the experimental results from AECL's Buffer/Container Experiment. A numerical analysis was carried out and the numerical results are compared against the experimental data. Further numerical investigation is launched to analyse the swelling phenomena observed at the buffer material and its effect on the Buffer/Container Experiment's behaviour. A conceptual model that describes the transient nature of the micro/macro behaviour of a swelling bentonite-based buffer material is presented. The model is incorporated into the numerical model and found to provide a good correlation with the experimental
results. Parametric studies on the buffer material’s saturated flow rate are also presented.

Chapter 7 describes the proposed geometry layout for an In Room Emplacement scheme. A numerical simulation of the proposed layout, including the transient micro-macro structure model described in Chapter 6, is presented and discussed. Several parametric studies on critical issues thought to affect the In Room’s performance are also presented.

Finally, Chapter 8 presents the conclusions obtained from the studies carried out, and suggestions are made for future research.

1.5 Reference


Chapter 1

Introduction

Figure 1.1  Schematic layout of AECL’s concept for deep disposal of nuclear waste (after Graham et al., 1997)
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Steel Sets for Ground Control
Invert Steel Structure
Gantry Crane Rail
Pressurized Water Reactor Waste Package
Codisposal Waste Package Containing Five High-Level Waste Canisters with One DOE Spent Nuclear Fuel Canister

Figure 1.2 An example of a horizontal canister deposition configuration (after Nuclear Energy Institute, 2004).
Chapter 2

Literature Review

2.1 Introduction

This chapter reviews developments made in the understanding and modelling of the thermal, hydraulic and mechanical behaviour of unsaturated soil. An overview is also presented on research related to the performance of high level nuclear waste repositories. This overview outlines the results and lessons learnt from the experiments carried out based on the concept of underground disposal.

In Section 2.2 research related to theoretical modelling of coupled heat, moisture and pore air transfer is reviewed. Section 2.2 also includes a review of the developments made on modelling deformation behaviour of unsaturated soil as well as the incorporation of deformation behaviour into existing thermal hydraulic theoretical models.

Section 2.3 considers the influence of the micro-macro structure of clay on moisture flow. This section takes a more detailed look at the structure of clay mineral and clay-water systems.

Section 2.4 reviews various modelling approaches that have been developed to simulate the micro-macro behaviour of swelling clay.

Section 2.5 presents a review on multi barrier systems proposed for underground repositories for disposal of high level nuclear waste. This is generally agreed by most countries as a long term solution for high level nuclear waste disposal.
Many experimental and numerical studies have been performed to improve the
design of a high level nuclear waste repository. Section 2.6 considers some of the
large scale experimental work associated with this problem. Numerical simulation
work, description of the results and correlation to the measured results are also
discussed.

Finally, conclusions from the literature review are presented in Section 2.7.

2.2 Developments on Theoretical Modelling of Unsaturated Soil

A review on recent developments made on the theoretical modelling of coupled heat,
mass and air transfer in a deformable unsaturated soil is presented in this section.
Initially, coupled heat, mass and air modelling for unsaturated soil is discussed. In
section 2.2.2, the developments made on the prediction of deformation behaviour is
highlighted. Finally in section 2.2.3, developments on theoretical models capable of
coupling both flow and deformation behaviour of unsaturated soil are presented.

2.2.1 Coupled heat mass and air modelling of unsaturated soil

Dakshanamurthy and Fredlund (1981) proposed a one-dimensional formulation for
coupled heat, mass and air flow in unsaturated soil. Three partial differential
equations were employed to describe all three flow phases in an unsaturated soil.
Fick’s law was used in the governing equation for air flow. Darcy’s law was applied
on liquid and water vapour flow. Both diffusion and advection effects were
accounted for in the formulation of water vapour flow. As for heat flow in
unsaturated soils, the Fourier diffusion equation was employed to include the effects
of conduction and latent heat of vaporisation. A finite difference scheme was
implemented to solve the three governing equations and the proposed model was
used to simulate the flow condition in compacted Regina clay. However, the
proposed model did not consider the coupling between heat and moisture transfer
and it was assumed that fluid permeability was constant. The model was applied to
several problems involving coupled flow in unsaturated soils under hydraulic and
temperature gradient. A reasonable match was obtained when compared against the
experimental results.
Couvillion and Hartley (1986) investigated the movement of thermally induced drying fronts in sandy soils and presented an explicit finite difference solution for the governing equations used to describe the flow of heat, moisture and air. The Philip and de Vries (1957) approach was used to represent liquid flow. Darcy's Law was used to represent the bulk flow of moist air mixture and Fick's Law was used to describe water vapour diffusion. However numerical difficulties were encountered. The air phase continuity equation was subsequently removed from the formulation and the heat transfer phase was simplified to overcome this problem.

Geraminegad and Saxena (1986) presented a mathematical model for the flow of heat, moisture and air transfer in unsaturated porous media. Three linear partial differential equations were derived. The heat and liquid flow were based on the modified Philip and de Vries approach, whilst gas flow was based on Darcy's Law. The effects of convection and latent heat of vaporisation were not modelled. However, the transfer of dissolved air and volume changes in the soil due to pore water pressure changes were included. A finite element solution was proposed for the mathematical model presented. Geraminegad and Saxena further simplified the solution by incorporating only two governing equations and omitting the air phase governing equation. The simplified model was then used to solve some case histories available in literature.

Whitaker (1977) applied the volume averaging method to provide a rational route to yield a set of equations describing heat and mass transport. He considered the effect of capillary action on moisture transport and derived a constitutive equation to describe the moisture movement. Pollock (1986) developed a mathematical model to describe the phenomenon of coupled energy, moisture, and dry air transport in unsaturated media. Three coupled non-linear partial differential equations were developed based on the Whitaker (1977) approach. A finite difference method was used to solve the governing equations. The model was used to simulate a hypothetical one-dimensional transport process in a large scale nuclear waste repository. Numerical results for liquid saturation, temperature field and air pressure distribution over a long period of time have led to the identification of important characteristics of air and water flow which have significant implications on radio nuclide movements.

2-3
Connell and Bell (1993a) developed a numerical model capable of predicting the influence of climatic change on moisture and vapour transport processes in waste dumps. Unlike previous approaches, thermodynamic equilibrium between liquid and vapour phases was not assumed. Liquid flow was described by Richard's equation, (Richards, 1931) which neglects the influence of thermal and air pressure effects on the liquid flow. Vapour flow was assumed to be formed by viscous vapour flux and diffusive vapour flux. Viscous vapour flux was described by Darcy's Law and the diffusive vapour flux was described using the dusty gas model (Thorntenson and Pollock, 1989). A moving node finite element solution of the coupled equations was then employed to analyse and solve the governing equations. Good agreement was found between the results from this model and those from alternative models when simulating isothermal infiltration into Yolo light clay. In a subsequent paper, Connell and Bell (1993b) applied a simplified version of the full model to simulate moisture movement in potential oil-shale dumps. A sensitivity analysis of moisture movement in a shale column and determination of relevant parameters were also carried out.

Thomas and Sansom (1995) proposed a theoretical model to describe the coupled flow of heat, mass and air in unsaturated soil. The air phase consists of a binary mixture of dry air and water vapour. The liquid phase is assumed to be water containing dissolved air. Three coupled governing equations were proposed where Darcy's Law was used to represent the liquid flow, the Philip de Vries approach (1957) to describe the water vapour flow. The influence of bulk air flow on the vapour flow, effects of conduction, convection and latent heat of vaporisation were all considered in this model. Spatial discretization was achieved by means of using the finite element method, and temporal discretization was achieved using finite difference technique. The model was used to simulate coupled heat, mass and air transfer in unsaturated sand. Good correlation was observed when the predicted results were compared against numerical results produced by an alternative model based on Pollock's work (Pollock, 1986).

Thomas and Ferguson (1999) presented a fully coupled heat and mass transfer numerical model that describes the migration of contaminated gas through an engineered clay liner of a sanitary landfill site. A mechanistic approach was adopted where mass and energy conservation laws are defined for a particular phase into
which Darcy’s and Fick’s Law are both substituted. This model treats the migration of liquid, heat, air and contaminant gas separately with independent system variables of capillary potentials, temperature, pore air pressure and molar concentration of the contaminant gas. The numerical results showed good agreement when compared against analytical solution obtained using classical advection-diffusion equation. The study also highlights the necessity of including the effect of a temperature gradient on the contaminant gas concentration.

Kanno et al. (1996) performed experimental and numerical investigations on moisture movement in highly compacted bentonite under temperature gradient. They assumed that the vapour flow area factor increases linearly as volumetric air content increase. Good correlations were observed when comparisons were made for the experimental and numerical results.

### 2.2.2 Developments on Modelling Deformation Behaviour in Unsaturated Soil

In recent years, much research effort has been directed to the coupling effects between the thermal, hydraulic and mechanical fields of unsaturated soil. This section sets out to highlight developments made on the theoretical modelling of deformation behaviour in unsaturated soils. A number of reviews are available in the literature on the deformation of unsaturated soils, (Alonso et. al., 1987; Hueckel and Baldi, 1990; Fredlund and Rahardjo, 1993; Delage and Graham, 1996; Wheeler and Karube, 1996; Sultan et. al., 2002). In view of the extent of information available in other literature, this section only intends to provide a brief summary.

Bishop (1959) proposed a theoretical model for simulating the deformation behaviour of unsaturated soil based on the effective stress concept;

$$\sigma^* = (\sigma - u_a) + \chi (u_a - u_i)$$

where $\sigma^*$ is the effective stress, $u_a$ is the pore air pressure, $u_i$ is the pore water pressure and $\chi$ is a parameter highly dependent on the degree of saturation, stress history and soil structure. The use of the effective stress concept to describe deformation behaviour of an unsaturated soil follows the basic assumption given by
Terzaghi (1936) that "all measurable effects of a change in stress... are exclusively due to changes in the effective stress ".

However, the use of the effective stress concept was met with limited success (Jennings and Burland, 1962; Bishop and Blight, 1963; Aitchison, 1965; Burland, 1965). Consequently, the focus of attention shifted towards using two stress state variables to describe the deformation behaviour of unsaturated soil. Coleman (1962) and Bishop and Blight (1963) suggested the use of net stress, \((\sigma - u_a)\), and matric suction, \((u_a - u_l)\), to describe the deformation behaviour. Matyas and Radhakrishna (1968) conducted a series of experiments on a mixture of flint powder (80%) and kaolin (20%), and proposed that the void ratio and the degree of saturation should be used to represent the deformation state of unsaturated soil. Barden et al., (1969) confirmed that a state surface is only unique for monotonic loading sequences.

Fredlund and Morgenstern (1977) conducted a series of tests and confirmed the ability of the stress state variables; net stress and matric suction, to describe the deformation behaviour of unsaturated soil. A third stress state variable, \((\sigma - u_l)\) was also put forward and it was proposed that any two of the three stress state variables could be used to form a suitable stress state system for unsaturated soil. Fredlund (1979) proposed a state surface defined by void ratio and gravimetric water content. These expressions have the capacity to include wetting induced swelling and collapse, on condition that the compressive indices have been defined as being stress dependent.

Lloret and Alonso (1980) developed a one dimensional consolidation model that includes a description of state surfaces for void ratio and degree of saturation. The proposed form of state surface for void ratio accounts for both wetting induced swelling and wetting induced collapse. A number of limitations could be identified with this approach. Firstly, the state surfaces did not include the influence of deviatoric stress on the deformation behaviour of soils; secondly, the state surfaces can only represent elastic deformation behaviour; finally, the uniqueness of the state surfaces can be ensured only if the monotonic load paths are followed. The limitations of elastic models can be overcome by the use of elasto-plastic models. These models are able to distinguish between plastic and elastic strains, as well as
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describing the links between volumetric and shear behaviour for both expansive and non-expansive soils.

The model presented by Alonso et al., (1990) represents a key development in the elasto-plastic modelling of unsaturated soil. The model has the capability to describe the stiffness change of the soil due to suction changes, the ability to simulate irrecoverable volumetric strains during the wetting collapse of the soil, and incorporate net stress for the evaluation of the rate of collapse. The model was based on the two independent stress state variables defined by Coleman (1962). An elastic region is bounded by a yield surface. The effect of shear stress on the state surface of the elasto-plastic model is defined using deviator stress. The isotropic stress state is derived using a yield locus in the net stress and the suction space, which can be further defined by two yield curves; suction increase curve (SI) and loading collapse curve (LC). For isotropic stress state a constitutive equation for a specific volume is defined, whilst a stiffness parameter for stress changes in the plastic region is defined as being a function of suction. An asymptotic expression was proposed to represent the increase in the stiffness of the soil with increasing suction.

Research conducted on the LC yield curve validates the model proposed by Alonso et al. (1990). Josa (1988) and Wheeler and Sivakumar (1995) proposed alterations to the mathematical formulation for the LC yield curve. Josa et al., (1992) included a maximum possible collapse on wetting in Alonso’s model. Wheeler and Sivakumar (1995) conducted a series of suction-controlled triaxial tests on compacted kaolin and proposed modifications on the number of suctions and the changing shape of the yield curve as it develops. Their experiments indicate that the normal compression lines are linked to the shape of the yield curve.

Alonso et al., (1995) performed a coupled flow-deformation analysis on an in situ isothermal wetting experiment. Two mechanical constitutive models have been used in the simulation: a state surface approach and an elastoplastic model. Predictions by both models have been compared against actual site measurement records. Encouraging correlations between the measured and calculated results were obtained. The state surface approach requires fewer parameters than the elasto-plastic model and they are more readily found. The authors added that the numerical results were critically dependent on some key parameters (e.g. hardening parameter) and they are
difficult to measure in practice. The state surface approach yielded results that failed to agree quantitatively with the measured value, especially with the time development of stresses. This was attributed to the apparently unrealistic continuous and rapid softening of the soil as hydration proceeds.

Cui et al., (2002) adopted some basic concepts from the model presented by Gens and Alonso (1992) and introduced the concept of critical swelling curve (CSC). The curve accounts for the couplings between hydraulic and mechanical effects. The non-linear model was found to provide satisfactory predictions of the volume change behaviour of heavily compacted swelling clays.

The inclusion of the suction increase (SI) yield curve in the model proposed by Alonso et al., (1990) was based on experimental evidence presented by Yong et al., (1971). Irreversible plastic shrinkage strains were produced during the drying-wetting cycle. The model proposed by Alonso et al., (1990) assumed that once the maximum allowable suction value is exceeded, irreversible strains are produced.

One of the earliest elasto-plastic models that takes into account the effects of temperature on the behaviour of soil was presented by Hueckel and Baldi (1990) where an increase in temperature corresponds to a decrease in volumetric yield. Sultan et al., (2002) extended the existing model to include additional plastic mechanisms to account for the effects of over-consolidation ratio (OCR) on the thermal expansion of contraction behaviour. A new thermal yield curve (TY) was proposed to allow for the generation of thermal contracting plastic volume changes, even at high OCR ratios.

Delage and Graham (1996) suggested that plastic hardening instigated by an increase in mean stress could result in microstructural rearrangements. Under constant pressure, the rearrangement would increase the suction values required for yielding to happen. A number of other elasto-plastic models have been presented in the literature that use stress state variables. Complex stress state variables were adopted to simplify the elasto-plastic formulation, (Karube, 1988; Kohgo et al., 1992; Kato et al., 1995)

Chiu and Ng (2003) developed a state-dependent elasto-plastic constitutive model for both saturated and unsaturated soils. The model, which is developed under an
extended critical-state framework, uses two independent stress state variables: normal stress and matric suction. In addition, the influence of a simplified non-linear soil water characteristic curve on mechanical behaviour is incorporated in the model by using a bi-linear function. A state-dependent dilatancy formulation is introduced to account for the effects of stress level or stress ratio, density and soil suction. The simulated results show that the stress-strain and volumetric shear-strain relationships at both loose and dense and saturated and unsaturated states can be modelled properly with a single set of parameters. The model is also capable of capturing some key observed features, such as a sudden increase in shear strain and volumetric strain as suction is reduced under a constant deviator stress.

Gallipoli et al., (2003) presented an elasto-plastic model for unsaturated soils that takes into account suction effects on soil's mechanical behaviour as well as suction’s dependence on the degree of saturation. The proposed model is formulated in terms of two constitutive variables directly related to these suction mechanisms: the average skeleton stress, which includes the average fluid pressure acting on soil pores, and an additional scalar constitutive variable, related to the magnitude of the bonding effect exerted by meniscus water at the inter-particle contacts. When the experimental isotropic compression data was analysed, the quotient between the void ratio, e, of an unsaturated soil and the void ratio corresponding to the saturated state at the same average soil skeleton stress, is a unique function of the bonding effect due to water menisci at the inter-particle contacts. Based on these observations, an elasto-plastic constitutive model was developed using a single yield surface. The model was able to simulate many important features (such as irreversible strain in wetting-drying cycles) of unsaturated soil behaviour. As a result of the behaviour normalisation achieved by the model, Gallipoli et al., (2003) believed that the resulting constitutive model is economical in terms of the number of tests required for material parameter determination.

2.2.3 Coupled thermo/hydro/mechanical behaviour in unsaturated soil

Previous sections have reviewed models that deal with aspects of flow and deformation in soils separately. This section reviews theoretical models which couple the flow and deformation behaviour of unsaturated soils.
Barden (1965) presented a consolidation model for unsaturated clay. The model is able to describe the pore water pressure, fluid conductivity, the pore air pressure and porosity. The flow through a soil is represented by Darcy's Law. However the flow of water vapour and dissolved air were not included in the model. An effective stress approach was used to represent the volumetric deformation (Bishop, 1960). The governing equations were solved using a finite difference scheme and the model was applied to a one-dimensional consolidation problem.

Later, Fredlund and Hasan (1979) presented a one-dimensional consolidation model. Basic concepts from Terzaghi's theory (Terzaghi, 1943) were modified and subsequently used to predict the vertical compression, whilst mass continuity was used to form equations for flow. When full saturation is reached, Terzaghi's equation returns to its original state. This model was subsequently used to simulate one dimensional consolidation problems.

Lloret and Alonso (1980) presented a one dimensional model for moisture and air flow through a deformable soil. They used the state surface approach presented by Matyas and Radhakrishna (1968) to represent the deformation. Net stress and suction were used as the stress state variables. Darcy's Law was used to represent the flow. Although dissolved air was included in this formulation, water vapour transfer was neglected. A finite element method was used to solve the governing equations, and the model was applied to swelling, loading cases leading up to a collapse in the soil system.

Chang and Duncan (1983) proposed a formulation to simulate flow and deformation in unsaturated soil. In their formulation, air and water in the soil were assumed to be represented by a homogeneous fluid. Effective stress was used as the basis in their elasto-plastic stress strain relationship. A finite element method was used to solve the governing equations, and the model was subsequently used to simulate the consolidation of an unsaturated soil under a strip footing.

A few years later, Edgar et al., (1989) developed a non-isothermal consolidation model using four governing equations to model the flow of liquid, vapour, air and heat through a deformable soil. The theory of mixtures was used to formulate the governing equation for energy balance, (Truesdell and Toupin, 1960). Thermal
deformation was neglected in the formulation. A finite difference method was used to solve the governing equations, and the model was used to simulate water content and settlement profiles in an unsaturated soil.

Thomas and He (1994, 1995) presented a coupled theoretical formulation to represent the thermo/hydro/mechanical behaviour of deformable unsaturated soils. The stress state variables of net stress and suction were used, and two constitutive models were developed. A non-linear elastic state surface model was presented by Thomas and He (1995), whilst an elasto-plastic constitutive model adopting the basic concepts in the model presented previously by Alonso et al. (1990) was presented by Thomas and He (1994). A finite element method was used to solve the governing differential equations and a finite difference method was used for the time stepping scheme. The proposed models have been used in a wide range of applications (Thomas and Zhou, 1995; Thomas et al., 1994a, 1994b; Thomas et al., 1998, Thomas and Cleall, 1999). Later the model presented by Thomas and He (1995) was extended for three-dimensional problem that allows greater complexity work to be analysed. Three-dimensional 20 node-isoparametric elements were used to simulate different types of cases for verification purposes. Good agreements were observed when the simulated results were compared against experiment results.

Yang et al., (1998) presented a 3-D mathematical model for coupled heat, moisture, air flow and deformation problems in unsaturated soil. Flow of pore water and air are represented by a generalized Darcy’s Law. They have considered movements of water vapour to occur due to molecular diffusion and as part of bulk flow of pore air. Fick’s Law is used to represent the molecular diffusion process. The effects of convection, conduction and latent heat of vaporization are also considered. A fully coupled, non-linear differential equation is established and solved using a Galerkin weighted residual approach in a space domain with an implicit integrating scheme in the time domain. Good agreement between the computed numerical results and the measurements of several cases from published literature were obtained.

Zhou (1998) presented a coupled non-linear model that accounts for thermo-osmosis and thermal-filtration in a fully saturated media. Zhou and his co-workers later presented a model to simulate coupled heat, moisture, and air transfer in deformable unsaturated porous media. Numerical solutions were obtained for heating,
infiltration, and loading of a soil column which demonstrate the principal features of coupled fields and experimental measurements were used to validate the model (Zhou et al., 1998). The model takes into account the effects of liquid flow on temperature gradient, heat flow on water potential gradient, temperature effect on void ratio, heat sink due to thermal deformation, compressibility of water, vapour, air and medium. However, the effect of hysterises is ignored.

Navarro and Alonso (2000) presented a comprehensive formulation for coupled thermo/hydro/mechanical phenomena in unsaturated soils. The model that can be used for expansive soils includes consideration for soil microstructure where a double structure formulation was used to model the fluid transfer between macropores and micropores. Their software, Flow and Deformation in Soils (FADES) allows alternative numerical strategies and contains a number of different constitutive equations for the various physical phenomena considered. FADES's elastoplastic model is derived from the model present by Alonso et al. (1990) which is also known as the Barcelona Basic Model (BBM). The model was validated against measured results and good agreement was observed when compared against the computed results.

Laloui and Modaressi (2002) presented a mathematical model capable of describing non-isothermal behaviour of saturated porous clays. Their thermo/hydro/mechanical (THM) formulation is derived on the basis of mass, energy and equilibrium equations formulated at the microscopic scale and averaged to the macroscopic scale using the homogenisation theory. The THM model is capable of taking into account the effects of thermal hardening and irreversible thermal strains.

Khalili and Selvadurai (2003) presented a fully coupled constitutive model for thermo/hydro/mechanical analysis in an elastic media with double porosity. The governing equations satisfy an effective stress concept; flow is described using Darcy's law, Fourier's law and the equations of Hookean thermoelasticity. The equations are derived using a systematic macroscopic approach that satisfies conservation laws applicable to the balance of linear momentum, mass and energy. Phenomena such as thermal expansion, thermal convection by moving fluid, heat flux due to pressure gradients and the heat of phase compression have also been accounted for.
Thomas et al., (2003) presented a paper which proposes a multi-level parallelized substructuring-frontal combined algorithm for the analysis of thermo/hydraulic/mechanical behaviour in unsaturated soil. Temperature, displacement, pore water pressure and pore air pressure are treated as primary variables in a non-linear analysis. The incorporation of the algorithm in a multi-level parallel strategy is found to be able to reduce both computer storage requirement and time needed for execution.

2.2.4 Conclusions

A review on recent developments made on the theoretical modelling of coupled heat, mass and air transfer in unsaturated soil is presented. In most coupled heat mass and air modelling, the Fick's law was used in the governing equation for air flow, Darcy's law was applied on water flow. Currently, theoretical modelling of flow and deformation behaviour of unsaturated soils is capable of modelling soil consolidation, elasto-plastic behaviour of soil, thermal hardening and thermal strains. In addition to that, researchers have begun looking at increasing the efficiency during execution and reducing the storage requirement.

2.3 Micro-macro structure and its role in clay matrix

An improved understanding of clay at microscopic level and the influence it has on the macroscopic behaviour is necessary to predict with greater confidence and accuracy the hydraulic behaviour in soils. However, before a descriptive macroscopic overview of clays can be derived, a clear understanding of the clay molecular structure and the physico-chemical forces involved is important. The following section presents the advances made on the identification of clay structures and the role of clay water interface.

2.3.1 Clay Mineral Structure

Pauling (1930) identified the existence of a multi-layer structure in clays which prompted the use of various modern tools such as X-ray, electron diffraction and nuclear magnetic resonance by researchers to obtain a clearer picture on the clay structure at microscopic (molecular) level.
According to Sposito (1989), clay minerals are aluminosilicates that predominate in clay fractions of soils at intermediate to advanced stages of weathering. Such clay minerals consist of layers of tetrahedral and octahedral sheets, superimposed in different ways. An illustration of typical tetrahedral and octahedral units is shown in Figure 2.1. Clay minerals can be characterized into groups known as kaolinite, illite and montmorillonite. Each type of clay is distinguished by the number of tetrahedral and octahedral sheets combined, as well as the nature of isomorphic cation substitution that occurs. Touret et al., (1990) identified several levels of clay structure organized in a hierarchical manner for the fabric units and pore spaces. Figure 2.2 extracted from an article by Yong (1999a) illustrates the hierarchical order of fabric units and pore spaces which clays are formed.

2.3.2 Clay-Water Interface

Central to a sound model capable of predicting the thermal, hydraulic and mechanical behavior in unsaturated soil is the understanding of the interaction developed by the interlayer and inter-particle forces in the presence of water, as well as the governing roles played by the unit layer separation (ULS), micropores and macropores. Interactions between fabric units and pores spaces within swelling soils govern the development of matric and osmotic forces. Both forces which account for the water uptake phenomena have been the subject of many research works.

Clay/water interaction has a tremendous influence on the clay's behaviour. According to Saiyouri et al., (2000), macroscopic swelling occurs at two microscopic steps. Initially, water is adsorbed between elementary clay layers. This is followed by filling up spaces of larger pore sizes. During the first step mentioned above, exposure to water results in penetration of water into the superimposed layers, thus forcing the layers apart. The force has been identified as *hydration force* (Yong and Warkentin, 1975; van Olphem, 1977). Many workers (van Olphen, 1977; Pusch, 1997; Alonso et. al., 1999) agreed that the interlayer swelling between clay and water could extend to a distance of four molecular layers of water. The hydration force causes water properties such as diffusion coefficient and viscosity, to vary with proximity from the clay layers. Baldi et al. (1988) observed that the thermal expansion for interlamellar water is significantly lower than that of bulk water. Figure 2.3 presents the change in
water properties away from the surface of montmorillonite surfaces (Ichikawa et al., 1999).

Observing Figure 2.1, clusters of hydrated clay platelets would form particles. Particles are an assemblage of stacked silicate layers and adsorbed water. An aggregation of such particles swells under hydration and shrinks under desiccation. Subsequent water uptake into the larger pore sizes is in response to the osmotic forces. Swelling of clay at microscopic level will eventually infringe into neighbouring pores and reduce their radii. According to Poiseuille’s Law, the rate of fluid flow through a circular pore is proportional to the 4th power of the radius of the pore. Consequently, the swelling reduces the permeability and also the convection transport of dissolved substance in water.

Many researchers [Pusch (1981); Low (1987); Yong (1999b); Saiyouri et al., (2000)] believe that the behaviour of swelling clays depends on the nature of exchangeable cations in the interlayer spaces and the initial water content of the partly saturated soil. At the same bulk weight and degree of saturation, Pusch (1980) found that 'illitic clay has interacting open voids, high flow capacity, but smectite was found to be more homogeneous, with smaller void and lower permeability value.' Yong (1999a) postulated that water movement in unsaturated soil was primarily in the form of film or boundary layer transport. Experimental research indicates that fluid transport in the larger pores do not exist in the absence of dominating external gradients because there is a lack of continuity between large pores and also only the internal driving forces respond to soil water potentials. Yong (1999a) also states that when equilibrium is reached, the osmotic potential (due to saturated micropores) is balanced by the matric potential in macro pores. Matric potential is a result of the microcapillary phenomena, van der Waals forces and weak osmotic phenomena. Pusch (1981) reported that the large reduction in the permeability for swelling clay is due to tortuosity. This statement lends support to the hypothesis by Yong et al. (1999a) on the idea that boundary layer transport is the dominant form of water flow.

Low (1980) found that the double layer (osmotic) component of the swelling pressure is negligible in clays. Experiments by Low (1987) concluded that swelling pressure is essentially independent of the specific nature (i.e. charge density,
geometry) of the clay and depends exponentially on the distance between superimposed layers of smectites. The same work also concluded that the thermodynamic, hydrodynamic and spectroscopic properties of water in clay-water systems differ from pure bulk water.

2.3.3 Conclusion

A review of the research work performed on the micro-macro structure of clay and its influence on the clay-water interaction is presented. Literature review has indicated the existence of a hierarchical order of fabric units and pore spaces for clays. The microscopic and macroscopic properties were found to be different for pure bulk water and adsorbed water.

2.4 Modelling Clay’s Behaviour

The description of flow and the modelling of the transport process in a multi-phase, heterogeneous system have received considerable attention from researchers all over the world. Investigations have also been performed to link the microscopic characteristics of the material (e.g. mineralogy, geochemical properties, structural components etc.) to its macroscopic behaviour (e.g. swelling, deformation, heat transfer). Researchers have also recognised the importance of achieving reasonable compatibility between the conceptual and the numerical models they choose to adopt.

A robust constitutive relationship that accounts for the description of the material properties as well as the morphology of constituent phases is crucial to model clay’s behavioural response accurately. In recent years, the phenomenological and micromechanical/homogenization approaches have emerged as the preferred methods within the framework of constitutive modelling of heterogeneous materials such as clays.

The following sections set out to highlight the advantages and disadvantages when using the phenomenological and homogenization approach. A literature review has also been performed on models that have adopted other approaches. The author has grouped these ‘alternative’ models and presented them in Section 2.4.3.
2.4.1 Phenomenological Approach

A number of researchers have used phenomenological approaches for solving multi-phase problem. Kattan & Voyiadjuis (1993) and Chaboche et al., (1994) believe that a generalization method is capable of formulating a good constitutive equation from the experimental results and the conclusion thereafter. From experimental observations, the derived phenomenological theories could introduce internal scalar and tensor variables, whose growth is determined using by appropriate evolution laws. Principles of irreversible thermodynamics, internal state variable theory as well as and relevant physical considerations are subsequently employed to describe an effective homogeneous material response. However, these models seemed to lack critical information (e.g. rate of adsorption and physico-chemical forces) on the micro-structural morphology and require many different experiments to evaluate the constitutive parameters for each different phase.

2.4.2 Homogenization Approach

In recent years, the homogenization technique has been adopted by many researchers when modelling heterogeneous material such as metal alloy systems, polymer blends, porous and cracked media. Homogenization as a method to determine the macroscopic overall characteristics of heterogeneous media is favoured as it provides a striking balance from time and cost view points. Besides that, the technique allows accurate predictions for the behaviour of unsaturated clay.

A straightforward experimental measurement on a multitude of material samples, phase properties, volume fraction and loading histories is hardly a feasible task. Due to the enormous difference in the length scales involved, it is impossible to generate a finite element mesh that can accurately represent the microstructure and also reach a numerical solution for the macroscopic structural component within a reasonable amount of time using state-of-the-art computational systems.

Hence, homogenization methods such as the rule of mixtures, effective medium approximation and asymptotic homogenization theory have been developed to obtain a suitable robust constitutive model at macroscopic level. These methods are based on the concept of a Representative Volume Element (RVE), introduced originally by Hill (1963).
Homogenization strategy works are based on a crucial assumption that heterogeneity for the material is very small compared to the body dimensions. Investigations by Schwier et al. (1985) and Dijkstra & Gaymans (1994) showed that the deformation field in the vicinity of one inclusion will be approximately the same as the deformation field near its neighbouring inclusions. Compatibility demands the two opposite edges and the two adjacent RVEs show identical deformations, where neither overlapping nor separation may occur.

Bowen (1982) utilised the theory of mixtures to formulate a compressible porous media model. His formulation allows for the effect of immiscibility and variable volume fractions. It also allows for the effects of pore relaxation by treating the volume fractions as internal state variables. This is particularly useful when attempts to describe the collapse of pore structures resulting from external loading are made. The macroscopic observation is such that the phases are seen as overlaying continua so that at each point, thermodynamic properties such as density, energy and momentum are defined spatially everywhere.

Work done by Bowen (1982) on the theory of mixtures has been modified and improvised by other fellow researchers. Achanta et al., (1994) proposed a three-spatial, single time-scale for moisture and heat transport developed for a multi-component, multi-phase unsaturated swelling porous media within the mixture theoretic framework. They assumed a scale separation where classical micro-scale theory of mixture was applied within each phase and interface. They postulated the existence of a two-scale hierarchy of overlaying continua, and that three distinct scales of motion exist in the multi-phase mixture. They have been identified as micro-scale (molecular), meso-scale and macro-scale.

According to a paper presented by Murad and Cushman (1997), a micro-scale comprises macromolecular structure of clay platelets polymer and vicinal fluid. They are considered to be non-overlaying continua, and occupy distinct regions of space and satisfy the classical field equations. These homogenized equations form an overlaying continuum with the intermediate (meso) scale using the hybrid mixture theory (HMT). At meso-scale, the homogenized swelling particles were mixed with two bulk phase fluids, i.e. bulk water and water vapour. At macro-scale, the homogenization procedure was repeated, forming four overlaying continua which
consist of doubly homogenized vicinal fluid, doubly homogenized macromolecules and singly homogenized bulk liquid and vapour phases. The three scale model is illustrated clearly in Figure 2.4.

For a clearer idea on the hybrid mixture theory (HMT), a brief summary of the key points is shown below:

- A methodical procedure for obtaining macroscopic constitutive restrictions which are thermo-dynamically admissible.
- Essentially a classical mixture theory applied to macroscale averaged balance laws for phases and interfaces. In this approach, the mixture of phases and interfaces are perceived as a set of overlaying continua.
- Constituents in the individual phases and interfaces are homogenized such that at each spatial point with the entire body, each phase, interface, and constituent possesses a continuous mass density.
- Constitution of the material at this macro-continuum scale is specified by listing a set of independent variables in terms of the macroscale properties of the system.
- Method aims to exploit the entropy inequality within the system.
- Three different phases (solid, liquid, and vapor) may be introduced and the macro-scale average independent variables are listed.

The theories were developed at meso-scale and macro-scale by exploiting the entropy inequality via the Coleman and Noll (1960) method, coupled with exchange transfer functions of mass, momentum and energy. Later, Murad and Cushman (1997) improved their existing model (Murad et. al., 1995) by incorporating the coupled effects of hydration, heat transfer and mechanical deformation. A modified Green’s function method was used to reduce the dual porosity system to a single porosity system with memory. The resultant theory provides a rigorous derivation of creep phenomena (delayed intra-particle drainage). The model also managed to reproduce the lumped parameter models for fluid flow, heat conduction and momentum transfer where the distributed source/sink transfer function is assumed proportional to the difference between the potentials in the bulk phase and swelling particles.
Eringen (1994) applied the theory of mixtures for porous elastic solids filled with fluid and gas, which included effect of heat conduction. Cook and Showalter (1992) extended the double porosity model (Yeh and Luxmoore, 1982) with microstructure that describes fractured porous media to include the case of partially fissure media, where a secondary flux effect arises from cell to cell diffusion paths. This refined model was thought to be advantageous as they include additional information associated with the fine scale structure of the fracture system. They believe that such ability was important even though fractures account for a very small fraction of the total volume, the bulk of the flow occurs at the fractures due to their high relative permeability.

Arbogast (1992) presented a model for a two-phase fluid flow in a highly fractured porous medium using a simplified dual-porosity approach. It was shown that the model was capable of modelling a two-phase incompressible flow of immiscible fluids in either an ordinary porous medium or in a naturally fractured porous medium. The equations were considered in a global pressure formulation that is justified by appealing to a physical relation between the degeneracy of the wetting fluid’s mobility and the singularity of the capillary pressure function.

Moutsopoulos et al., (2001) proposed using a multiple porosity continuum model to describe the hydraulic behaviour and contaminant transport in soil. They considered that the conditions are such that a horizontal 2D flow takes flow. By writing the continuity of mass (including exchange terms between the various families of fractures) and Darcy’s law for each family of fractures, macroscopic equations for both confined and unconfined flow are obtained. A classification procedure and geometrical idealization of the individual fractures for each family is proposed which enables the calculation of the exchange coefficients. Equations for the description of the contaminant transport in the field scale for both confined and unconfined aquifer are subsequently developed. Numerical investigations of representative problems have offered some insights into the behaviour of double and triple porosity aquifers.

Ichikawa et al. (1999) proposed using the unified method of molecular dynamics (MD) and homogenization analysis (HA) procedure to relate microscopic characteristics to an overall macroscopic behaviour. Their results were comparable to some existing experimental data. The unified 'molecular dynamics/homogenization
analysis’ (MD/HA) method was able to model micro non-homogeneous materials by providing an integrated procedure to simulate the molecule level and the macro-continuum behaviour in a seamless manner. The molecular dynamics process is capable of evaluating micro-scale material properties and statistical thermodynamics. The homogenization analysis procedure applies the mathematical perturbation method to extrapolate the behaviour of micro-inhomogeneous continuum to bulk-scale continuum.

The unified method of MD/HA analysis is also capable of developing a crystal model for montmorillonite with surrounding water. After specifying the inter-atomic potential functions for each atomic pair, the molecular dynamics computation can be performed. By applying a standard procedure of statistical mechanics to the molecular dynamics results, the bulk properties (swelling properties, shearing viscosity, bulk/vicinal water viscosity) of the swelling clay at the clay minerals’ neighbourhood can be defined. Finally, the macro-mechanics field can be determined using a homogenization analysis procedure where the properties of each constituent material are known. This unified molecular dynamics/HA concept can be extended to different classes of problems for the bentonite clay such as mass transport, moisture and water transport under unsaturated condition, thermal transport, time dependent deformation and failure.

2.4.3 Other Approaches

Emerman (1995) used a tipping bucket model to predict the flow in macropores within a porous media. He assumed that the macroporosity is equivalent to the saturated water content by taking off the field capacity. When the micropores are saturated, the field capacity has been reached and macropore flow occurs. However, it was noted that the tipping bucket model requires a suitable range of time step for its analysis.

In 1982, Yeh and Luxmoore (1982) applied a domain concept to simulate water flow and chemical transport in macro-mesopore systems. Two models were presented; single continuum approach (SCA) and double continuum approach (DCA). The first approach caters for situation when detailed spatial distribution of macropores can be mapped. The second approach however applies only when statistically averaged
distribution of macropores is available. Both approaches are found to be capable of simulating fast water movement and speedy chemical migration via available routes in the macropores. The simulations show that the macropores can increase the interactions of any incoming water and chemicals with the soil profiles. Besides that, the macropores are thought to provide better drainage, delay the onset of lateral flow and surface runoff process, as compared to a soil profile ‘without’ provision for cracks and channels.

Buyevich (1995) presented a theoretical model on joint filtration flow of immiscible incompressible fluids. His model accounts for the relaxation process via exchange of fluids between pores of different sizes, driven by capillary forces. The model developed is based on a crucial presumption that phase permeabilities for all fluids as well as the capillary pressures at interface separating them are single-valued functions.

Cerrolaza and Delage (1997) presented a model based on an experimental observation of the microstructure in soft clays and the Boundary Element Method (BEM). The matrix is considered to be linear elastic and obeys a Tresca failure criterion. The pore size distribution follows a Gaussian normal law. When a failure criterion is activated, (i.e. pore collapse) a non-linear analysis process begins.

Anandarajah and Chen (1997) conducted a study on synthesizing particle-level physico-chemical theories and arrived at a generalized macroscopic behaviour of an assembly of clay particles. They have used a non-linear optimisation technique with energy minimization.

Gens and Alonso (1992) proposed an elasto-plastic model for expansive soils. Alonso et al., (1994) made further improvement to the model two years later where mechanical coupling between micro and macrostructure are included and defined by two functions; one for wetting and the other for drying. They postulated that the change in macro-structural void ratio is dependent on the change in micro-structural void ratio, and their respective values depend on the state of compaction in the macro-structure. Phenomena such as the dependency of strain on stress-suction path, accumulation of strain during suction cycles at high/low confining stress, macro-pore invasion by expanded microstructure and changes in macro-porosity during strong
drying as well as secondary swelling can be represented. They have expressed the increments of volumetric macro-structural plastic strain due to micro-structural swelling/shrinkage by two coupling functions that depend on the ratio of mean net stress over pre-consolidation pressure. In another journal, Alonso et al., (1995) reported that soil density influences the magnitude of swelling. Swelling strains in a wetting path were also thought to depend on the initial water content and the applied confined stress. Their elasto-plastic model are based on research work published by Warkentin et al., (1957) which assumes that micro-structural volumetric deformation is reversible.

2.4.4 Conclusions

This section completes the review for the micro-macro structure in swelling clay and the approaches used to model the swelling clay’s behaviour. Microscopic behaviour of clay is determined at the micro-structure level where molecular bonding and ionic exchange play a pivotal role in defining the physico-chemical forces that exist at the microscopic level. This has a significant effect on the macroscopic parameters of swelling clays such as the hydraulic conductivity, tortuosity and soil density. Phenomenological and homogenization approaches are preferred by researchers to model the micro-macro behaviour in swelling clays.

2.5 Overview of High Level Nuclear Waste Disposal Repositories

Disposal of high level toxic nuclear waste poses an obvious health threat, and the manner that it is conducted requires thorough scientific investigation, to ensure that all possible worst case scenarios are avoided during the life time of the disposal unit. This section sets out to provide a concise overview on recent major developments that have occurred in the design of underground waste repository.

Many countries around the world have initiated extensive studies into the disposal of nuclear waste. After considering many options, deep underground repository is considered to be the best solution for disposal of high level nuclear waste. The variety of studies include the characterization of waste material and site storage location, modelling the interaction between engineered buffer and host rock, testing the durability and integrity of engineered barrier system, safe and efficient way of grouting and sealing techniques and post-closure monitoring systems. A thorough
understanding on the complex nature of deep geological disposal is necessary before
government, organisations and most critically the public can be convinced that a
commercial repository is viable and presents itself as the best option to safely dispose
high level nuclear waste. Low level radioactive waste was disposed of in Germany in
deep underground caverns in the Asse salt mine (1967-1978), and in a salt dome at
Morsleben since 1981, at depths exceeding 500 metres (Berg et al., 1997). In the
USA, the world’s first purpose-built deep geological repository for long-lived wastes
(excluding high-level, heat-generating wastes) has been operating at the Waste
Isolation Pilot Plant (WIPP), at a depth of 650 metres below ground in a bedded salt
formation in south-eastern New Mexico, since March 1999 (Riotte, 2000). However,
the United States of America has a near term timetable for high level nuclear waste
repository scheduled for operation in the Yucca Mountain, Nevada, by year 2010
(Artur, 2002). In Finland, Norway and Sweden, underground repositories for low
and medium level waste are operating at intermediate depths between 50 and 100
metres, at the Olkiluoto nuclear site (since 1992), at the Loviisa site (since 1998), at
Himdalen (since 1999), and at the Forsmark site (since 1988) (Riotte, 2000). It is
thought that the construction of a repository in Sweden could start by 2008 (Hogberg
et al., 2002). In May 2001, Finland became the first country to approve plans for a
geologic repository. The Finnish waste-disposal company Posiva Oy will research
possible sites and plans to start building the repository in 2010. However, the
repository is not expected to begin operation until year 2020 (NEA, 2000).

There are many research facilities around the world dedicated to the development of
the concept of underground waste repository. Although the ideology and disposal
concept from countries (e.g. United Kingdom, Japan, Sweden, Canada, USA etc.)
researching on waste disposal may differ, a common ground has been reached with
regards to the definition of geological disposal for high level nuclear waste. The
definition as well as the material composition in a typical geological disposal is
discussed in the following section.

2.5.1 Geological Disposal

"Geological disposal is provided by a system that will isolate the wastes from the
biosphere for extremely long periods of time and ensure that residual radioactive
substances reaching the biosphere will be at concentration that is insignificant
compared, for example, with the natural background levels of radioactivity.” (Nuclear Energy Agency, 1995). The majority of high level nuclear waste disposal units rely on a multi barrier system to isolate the waste from the biosphere. This multi barrier system typically comprises the natural geological barrier provided by the repository host-rock and its surroundings, as well as an engineered barrier system. This combination creates an overall robustness in the system. Further details on engineered barrier and the natural barrier system are discussed in the following sections.

2.5.1.1 Buffer materials
A review on available literature indicates much research work has been performed on the design for modern engineered barrier systems and the compatibility of the soil components within the system. The geological time-scale of the radioactivity arising from the nuclear waste means that in the likely event of slow disintegration of the waste canister, the engineered barrier has to be ready to with-hold the spread of the waste and to prevent any radio nuclide leakage into the biosphere.

Swelling clays from the montmorillonite group have been identified as the preferred material for engineered barriers in many concepts. Its unique engineering properties improve the performance of a barrier system (Felix, et al., 1996). In a densely compacted state, its low permeability slows down the movement of water and pore air, thus delaying the arrival of ground water to the canister which would initiate corrosion to the canister. Besides that, montmorillonite clay’s high surface area lead to a high sorption capacity, which means that it can act as a chemical buffer by delaying the transport of chemicals and radionuclides to groundwater. Furthermore, in case of any fracture (especially at the buffer-granite interface) which may occur due to the high temperature generated by the radioactive decay, montmorillonitic clay would tend to naturally seal up the fractures in the presence of water.

2.5.1.2 Natural Barrier Systems
A proposed construction site for an underground repository that contains the actual geological formations is known as the natural barrier system. These natural barrier systems can be hard rock, clay or salt, and provide the final protective barrier to prevent radionuclide emission. It is important that during the construction phase of the storage caverns the geological barrier must not be altered in a significant manner.
(NEA, 1994). An example of this is the amount of fracturing and cracking due to the drilling process should be minimised, as well as any chemical alterations from the construction process. Their engineering, chemical and other inherent properties are important in determining the suitability of sites for the positioning of deep underground geological repositories (Langer, 1998). Current geological and geophysical data make it possible to evaluate in detail the proposed sites, with the objective of providing studies of neotectonics, thermal properties of rocks, their hydrogeology and seismicity, to help researchers and engineers determine the most suitable host material as well as the site location (Galetsky et al., 1996).

2.6 Experimental Laboratory Research Associated with High Level Nuclear Waste Repository Development

Experiments linked with improving the design for underground nuclear waste repository play an important role in helping researchers obtain quality information regarding the material parameters, the thermo/hydro/mechanical behaviour of the buffer material and the host rock’s response, as well as the coupling effects and interactions between both materials. The experimentally obtained information is also very useful for validating numerical models. Good agreement between the numerical and experimentally measured results would increase the confidence on a numerical model, which could then allow researchers to predict a repository’s performance with greater accuracy.

There are different orders of experiments that can be carried out. Laboratory bench top experiments, large-scale mock-up experiments and large-scale in situ experiments are the types of experiments that have been performed. Mitchell (2002) reviewed some laboratory bench top experiments and these will not be repeated here. The following sections review some important large scale mock-up and in situ experiments that have been carried out over the past few decades.

2.6.1 Large Scale Mock-up Experiments

This type of experiment sets out to simulate the behaviour of buffer material in a borehole emplacement environment. By subjecting the experiment to well defined boundary and initial conditions, many uncertainties associated with a typical large scale in situ testing can be taken out, thus leading to a more accurate numerical
modelling of the experiment. Table 2.1 presents a summary on large scale mock-up experiments that have been performed and the comparison between the experimentally measured and numerical results.

2.6.1.1 Conclusions

Comparisons between experimental results and numerically modelled results show good agreement in the temperature, indicating that this field is well understood. The numerical models used are capable of making blind predictions of experimental work for the temperature variation.

However, simulations of the hydration behaviour in the bentonite by numerical models show discrepancies when compared against measured results. High levels of uncertainties were also observed for the stress and strain components in bentonite when numerical models were used to predict the mechanical responses in the experiments. Despite being tightly controlled experiments, the scale of such experiments inevitably introduces uncertainties that have yet been considered in the numerical simulations. Nevertheless, numerical modelling presents an option to investigate how soil would behave under different near field conditions in an almost real situation.

2.6.2 Large scale in-situ experiments

This type of experiment poses the most difficult challenges for any numerical modelling research group where the reliability and robustness of the model will be fully tested. A good numerical model should be capable of predicting the actual response in an experiment. The experimental results obtained from a large scale in situ experiment can be used as benchmark or back analysis exercises. The following section highlights some of the large-scale in situ experiments that have been performed in the past.

2.6.2.1 Large scale tests conducted as part of a benchmarking exercise

The hypothesis that the transport of radionuclides through barriers takes place only by diffusion requires confident estimation of the changes in the unsaturated clay barriers in a geological time scale. Several projects have been initiated to test numerical models which are able to predict the coupled thermo/hydro/mechanical
processes through an unsaturated clay barrier. Some of the important projects are highlighted here.

2.6.2.1.1 DECOVALEX

Development of Coupled Models and their Validation Against Experiment (DECOVALEX) is an international co-operative research project aimed to improve the understanding of various thermo/hydro/mechanical processes and how they can be described using mathematical models (Stephansson et al., 2001).

The DECOVALEX project was divided into three stages. DECOVALEX I studied a number of hypothetical benchmark tests, small scale laboratory experiments and large scale in situ experiments. DECOVALEX II focused on two large scale experiments whereas DECOVALEX III attempted to model large scale buffer mass experiment FEBEX at Grimsel test site in Switzerland, the Drift Scale Heater Test in Yucca Mountain at the Nevada Test Site and three more benchmark tests relating to re-saturation, upscaling, and glaciations.

Research teams from selected countries used their numerical codes to study the bench-mark test and test case problems in DECOVALEX I. Jing et al., (1996) found that most of the numerical models displayed fairly good agreement with the field test data. The quantitative discrepancies among the modelling teams could be accounted for by different choices of initial hydraulic aperture and joint normal stiffness.

The findings from DECOVALEX I shifted the focus of the project and two major large-scale in situ experiments were studied (Stephansson et al., 2001). A four point tasks had been defined for the DECOVALEX II; a numerical study of Nirex's Rock Characterisation Facility shaft excavation at Sellafield, United Kingdom, a numerical study of a THM experiment in Kamaishi Mine, Japan, a review of the state-of-art of the constitutive relations of rock joints and finally compiling a report on the understanding of coupled THM processes related to design and performance assessment of radioactive waste repositories.

For the Sellafield project, there were large discrepancies between the numerical results and the experimental results. Research teams that used axisymmetric models
Knight (2001) thought that it would have been useful if one or more of the research teams had modelled the fractured rock using a discontinuum approach, for comparison with the equivalent continuum approaches. Stephansson et al. (2001) thought that this test highlighted the importance of a prediction-calibration procedure in the prediction of the hydro/mechanical response to shaft sinking. They also found that treating the hydrological and mechanical responses separately was significantly easier than coupling the processes in a realistic in situ experiment.

2.6.2.1.2 CATSIUS CLAY
The European Commission formed a research programme on Nuclear Fission Safety where one of the projects was the CATSIUS CLAY project (Calculation and Testing of Behaviour of Unsaturated Clay as a Barrier in Radioactive Waste Repositories) which took place over a period of 3 years. The benchmark test set out to assess the accuracy and reliability of numerical predictions and find out more on the usability and capability of codes to model the thermo/mechanical behaviour of unsaturated clay barriers (Rees and Thomas, 1996). Research teams from all over Europe were invited to participate.

The CATSIUS CLAY project consisted of three stages. In the first stage verification of the code was conducted where two tests were considered; infiltration in a finite column of an unsaturated porous medium, and thermal convection in a saturated rigid porous medium (Alonso and Alcoverro, 1999). During the second stage the codes were validated against laboratory experimental results from oedometer suction controlled tests on samples of compacted Boom bentonite, and a small scale wetting/heating test on compacted bentonite (Alonso and Alcoverro, 1999). In the third and final stage, two large scale experiments were considered; the FEBEX heating-wetting mock-up experiment and the BACCHUS 2 in situ experiment. The FEBEX experiment has been presented previously in Table 2.1. The BACCHUS 2 in
situ experiment was performed at the HADES underground laboratory at Mol, Belgium. This in situ isothermal wetting experiment was designed to demonstrate and optimise an installation for clay based material and to study its hydration response (Alonso et al., 1995). The test was instrumented to allow the results to be used for validation of numerical models. Total stress, pore water pressure and water content measurements were taken in the backfill material and the host clay. The location, set-up and positioning of the instruments are shown in Figure 2.9.

Alonso et al., (1995) presented results from the first phase only. They used the results from the BACCHUS2 analysis to validate two alternative hydro/mechanical models: a state-surface approach and an elasto-plastic approach. They found that one of the advantages for the state surface approach was that it required fewer parameters that were more readily obtainable than the parameters needed for the elasto-plastic approach. They have also found that the predictions by the models were different both quantitatively and qualitatively. The in situ experiment has highlighted the difficulties in achieving homogeneous conditions in all the materials used.

2.6.2.1.3 INTERCLAY II

In the late 1980's, three modelling organisations conducted a finite element simulation based on experimental data from a Boom clay, provided by Mol/Dessel, Belgium (Knowles et al., 1996). This project was known as INTERCLAY I. The numerically modelled results among different organisations were quite similar, and these simulations encouraged CEC to conduct more comprehensive benchmark experiments. Hence, INTERCLAY II was earmarked to improve predictions on more realistic and complicated large scale experiments.

INTERCLAY II consists of three stages. In the first stage analytical solutions were solved in order to verify the numerical codes. Simple laboratory experiments were then modelled in the second stage, as a validation exercise. Finally the numerical codes were applied on to in situ experiments, and comparisons were made against the experimental results. These were blind predictions as results from the experiments were withheld from the participants.

The results from the verification exercise in stage one showed good agreements among the organisations, and against the analytical results. Two laboratory
experiments were performed and their results were used to validate the numerical codes in the second stage. The first was a heated triaxial test on kaolin clay samples. The participating organisations were given the experimental results for two triaxial tests and asked to back-fit their results to these values. Following that, they were asked to blindly predict numerical results for a third triaxial test. The temperature profiles were well matched for the three experiments, however the numerical pore water pressure profiles were consistently lower than the experimental results for the third test. The discrepancy may have arisen as the first two tests were undrained, whilst the third test was drained. Hence, the organisations did not have sufficient information to calibrate their models.

The second validation exercise for phase two of the benchmark test was a series of heated hollow cylinder tests supported by triaxial tests on Boom clay. The participants were asked to calibrate their models using the experimental results from the triaxial tests, and then blindly predict the results for the hollow cylinder tests. After analysing the results from the blind prediction, the participants were given the experimental results to enable a back-fitting exercise to take place. Discrepancies between the participants still exist for the volume change results. However a better agreement was achieved for the height variation and pore water pressure results.

At the end of stage two it was thought that the results demonstrated the difficulties of providing enough detailed information to adequately calibrate the numerical models, and that recognition was needed of the effects of anisotropy at laboratory scale (Knowles et al., 1996). Further work was recommended to further define the role of laboratory tests for calibration.

2.6.2.1.4 Mol/Dessel Nuclear Site, Belgium

The Mol/Dessel nuclear site in Belgium conducted several in situ tests (Bernier and Neerdahl, 1996). The BACCHUS test (BACkfilling Control experiment for High level wastes in Underground Storage) was conducted as part of the CATSIUS CLAY benchmarking exercise. The other tests performed were the CERBERUS Experiment and the CACTUS Experiment. Both experiments will be described in the following sections.
2.6.2.1.5 The CERBERUS Experiment

The CERBERUS (Control Experiment with Radiation of the BElgian Repository for Underground Storage) was developed under contract with Commission of the European Communities (CEC) and The National Agency for the Management of Radioactive Waste and Fissile Materials (ONDRAF/NIRAS). This experiment had a much longer time scale than the BACCHUS experiment which was carried out over a period of 5 years. The temperature and radiation effects were subsequently simulated. The experimental layout is illustrated in Figure 2.10. The sources were emplaced in October 1989, and power was activated in November 1989. Power shutdowns were experienced during the course of the experiment, and Bernier and Neerdael, (1996) made a few observations on the responses of the pore water pressure in the host clay. They found that the pore water pressure drops following a power shutdown but subsequently increases to the same or higher level. Besides that, the pore water pressure is more sensitive to a power shutdown, than the temperature within the clay. In addition to that, permeability decreases after a thermal load. The pore water pressure in the Boom clay was simulated using the TEMPRES program. It was found that good correlation can be observed between the numerically modelled results and the experimental results (Bernier and Neerdal, 1996). However, they conceded that the dissipation of the pore water pressure as micro-cracks began to appear in the Boom clay could not be reproduced using the code.

2.6.2.1.6 The CACTUS Experiments

The CACTUS Experiments were conducted to improve the understanding of hydro/thermo/mechanical behaviour of clay. More instruments that allowed the effective stress to be evaluated were installed in the experimental set up than in the BACCHUS or the CERBERUS experiments. Several conclusions were drawn from the CACTUS experiments (Bernier and Neerdal, 1996). They found that the heating created a rapid increase in the pore water pressure, which then dissipated towards a steady value. During the cooling stage, the pore water pressure decreased rapidly before reaching steady state.

Besides the CERBERUS and CACTUS experiments, two more thermo/hydro/mechanical tests were carried out at the Mol/Dessel nuclear site; ATLAS (Admissible Thermal Loading for an Argillaceous Storage) for which the
heating phase was started in 1994, and PRACLAY (PReliminary demonstration test for Clay disposal of highly radioactive waste). ATLAS was designed as part of a benchmark test (INTERCLAY II) to compare against the numerical results obtained. As for PRACLAY, it was designed to simulate a retrievable disposal scheme.

Both ATLAS and PRACLAY exhibited similar patterns of behaviour as the CERBERUS and CACTUS experiments (Neerdael and Volckaert, 2001). During the heating stage, the pore water was thought to expand, resulting in a rapid increase in total stress and pore water pressure level. A decrease in the rate of flow and water content, as well as an increase in the density and temperature was recorded during the heating phase. During the cooling stage, it was observed that the water content began to increase whilst the density of soil began to decrease. Neerdael and Volckaert (2001) concluded that the numerical modelling of the experiments carried out at Mol, Belgium was unable to fully capture the complexity of the clay behaviour. The inadequacies discovered from the numerical models would be useful in the future where the models can be further improved to produce better predictions.

2.6.2.1.7 Aspo Hard Rock Laboratory, SKB, Sweden

Svensk Karnbranslehantering AB (SKB) is responsible for all the handling, storage, transport and disposal of Sweden's radioactive waste. SKB has developed a research and development programme which includes the Aspo Hard Rock Laboratory (HRL) (Ericsson, 1999). The laboratory in Oskarshamn comprises a tunnel that is approximately 3600m long and descends to a depth of 460m. The research facility is located in the vicinity of the Oskarshamn nuclear power station. As the repository concept has to adapt to the overall geologic and tectonic conditions of its home nation, SKB considered deep disposal in an excavated vault at approximately 500m depth into crystalline rocks to be ideal.

The Aspo HRL provides an opportunity for research and development in a realistic and undisturbed rock environment. Tests and experiments have been carried out since 1995. According to Ericsson (1999), these experiments and demonstrations include Zone of Excavation Disturbance Experiment (ZEDEX), Tracer Retention Understanding Experiment (TRUE), Redox Experiment in detailed scale (REX), degassing and two-phase flow, Backfill and Plug Test, Prototype Repository and Long-term Tests of Buffer Materials (LOT). Among the listed experiments that have
been carried out, the Prototype Repository Project was able to provide an opportunity to investigate the feasibility of integrating various repository components and also to provide a full-scale reference for comparison with models and assumptions. The Prototype Repository is envisaged to be capable of simulating a real deep repository system. Instrumentations were used to monitor processes and physical properties in the canister, buffer material, backfill and the near-field rock. The experimental results can then be compared against results obtained based on conceptual and theoretical models. The prototype repository is being kept in operation for 20 years, although an extension to the length of the experiment is still being considered.

2.6.2.1.8 Atomic Energy of Canada Limited (AECL)

Atomic Energy of Canada Limited, also known as AECL, performed several large scale in situ experiments to investigate the interactions between a montmorrillonitic-type of clay and a host granite rock. These include the Isothermal Experiment, the Buffer/Container Experiment and the Tunnel Sealing Experiment (TSX). These experiments were performed at AECL's underground research laboratory in Manitoba, Canada.

The Buffer/Container Experiment involved the placement of a heater in a 5 m deep borehole drilled at the 240 m level of AECL’s underground research laboratory. The heater was surrounded by compacted buffer material in direct contact with saturated rock. The buffer and the rock were extensively instrumented to record the temperatures, suctions, and deformation within the buffer and the rock. The aim of the experiment was to assess the thermo/hydraulic/mechanical responses of the buffer at full scale in a realistic setting. Both the Isothermal Experiment and the Buffer/Container Experiment were carried out around the same period.

Initial studies of the Isothermal Experiment showed that an excavated damage zone (EDZ) was important prior to the placement of the buffer material within the borehole. During the experiment, the buffer would expand and seal the fractures in the rock. Mitchell (2002) reported that an exponential form of hydraulic conductivity relationship was capable of producing an improved set of correlation against the experimental results. In the Isothermal and Buffer/Container Experiment, swelling was also thought to have taken place in the buffer/rock interface and affected the
resaturation processes. Preliminary numerical investigations on both large scale experiments have shown reasonable representation of the actual behaviour.

The Tunnel Sealing Experiment (TSX) was performed at the 420m level of AECL’s Underground Research Laboratory. The experiment comprised two bulkheads, one composed of high performance concrete and the other of highly compacted sand-bentonite material. A permeable sand fill was installed in the chamber between the two bulkheads. The experiment is divided into two distinct phases. In the first phase (commenced immediately after the bulkheads were constructed) the sand chamber was incrementally pressurised with water at ambient temperature up to 4 MPa pore water pressure. The performance of each bulkhead under hydraulic flows was monitored and evaluated. In the second and final stage heated water was circulated through the sand chamber to evaluate the performance of the bulkheads and host rock based on the influence of elevated temperatures in the sand chamber.

Didry et al., (2000) used a numerical model that is based on the CESAR-LCPC Finite Element code to predict the behaviour of a concrete bulkhead. Prior to the actual experiment, it was predicted that a gap of 0.5mm would be developed between the bulkhead and the rock. Thomas et al., (2003) used a numerical model named COMPASS to perform a series of coupled and uncoupled thermo/hydro/mechanical simulations on the TSX experiment. Both 2-D axisymmetrical and 3-D analyses have been simulated. The numerical simulations have indicated that the clay bulkhead would completely resaturate after 3 years. In the THM simulation of Phase 2 it was found that the thermal expansion in the clay bulkhead had a notable effect on the pore water pressure distribution. The surface of the steel plate was simulated to have deformed by 8 mm in the simulation by the end of Phase 2.

2.6.2.2 Conclusions
An overview on the progress made on large scale in situ experiments and the modelling work performed has been presented. These in situ tests have provided valuable information to increase the confidence in the numerical models, to recalibrate these models and to improve our understanding on the thermo/hydro/mechanical interaction between existing components in each experiment.
Despite the improvements made on the modelling of thermo/hydro/mechanical behaviour in large scale experiments, certain shortcomings still exist and affect the level of confidence on the numerical models’ ability to produce accurate predictions. It is thought that the thermal behaviour is well understood and can be predicted to a high level of accuracy. However, there is an evident lack of understanding on the hydraulic interaction between the buffer materials and the host rock, especially at the interface between the two. As highlighted in the CERBERUS experiment, the dissipation of pore water pressure (due to the appearance of micro cracks) could not be reproduced in the numerical model (Bernier and Neerdal, 1996). As such, further research into the hydraulic interface is clearly needed. In addition to that, an accurate representation of the initial water pressures as well as the ability to model the transient changes in the hydraulic fields are thought to be important in order to reproduce the behaviour expected in an actual experiment from the numerical model.

2.7 Conclusion

This chapter firstly reviewed developments made on the theoretical modelling of the thermo/hydro/mechanical behaviour of unsaturated soil. It was found that the most widely used stress state variables used to represent the mechanical behaviour of unsaturated soil are net stress and suction. Most workers use Darcy’s Law to represent the flow of moisture, Fick’s Law to model the flow of pore air and Philip and de Vries (1957) approach to model the transport of water vapour. A number of constitutive relationships have been proposed to represent the elasto-plastic deformation behaviour of unsaturated soils.

A review was also made on the micro-macro structure of swelling clay (montmorillonitic group). At microscopic level, the interlamellar and clay layers are shown to affect the macroscopic overall behaviour of swelling clay. Adsorbed water and free water were found to have different engineering properties. Besides that, different methods of modelling clays’ behaviour (including the phenomenological approaches and the homogenization approaches) were described.

The current status of research into high level nuclear waste disposal was also reviewed. The concept of deep geological disposal using multi barrier system has been adopted by many countries as the preferred solution to the waste problem.
Different types of laboratory research work linked to the development of high level nuclear waste repository have been performed. Several large scale experiments have been carried out and numerical models have been used to predict the temperature and moisture field in the experiments. Comparison between measured and numerical result shows that the temperature field is well understood. However, more work is needed to improve the understanding of the moisture and the mechanical behaviour in a multi barrier system.
2.8 Reference


Chapter 2


Chapter 2 Literature Review


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Chapter 2  


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<th>Experiments</th>
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<td><strong>Commissariat a l’Energie Atomique (CEA)</strong> (layout refer to figure 2.5)</td>
<td>Heating experiment to investigate the difference in temperatures between the internal and external edges of the barrier. Isothermal experiment to investigate the hydration of the barrier.</td>
<td><strong>Heating Experiment</strong>&lt;br&gt;The heat energy arising from the convection process was underestimated.&lt;br&gt;A quarter of the water evaporated from the clay was found condensed on the walls of the equipment, producing swelling which fills up the voids. <strong>Isothermal Experiment</strong>&lt;br&gt;Saturation of the external surfaces of the clay kept the air from escaping from the blocks. The build-up of air pressure significantly slowed down the hydration process (Felix et al., 1996)</td>
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<tr>
<td><strong>Full-Scale Engineered Barriers Experiment in Crystalline Host Rock (FEBEX)</strong> (layout refer to figure 2.6)</td>
<td>A full scale experiment in situ test in natural conditions&lt;br&gt;A ‘mock-up’ test at almost full scale&lt;br&gt;A set of experimental laboratory tests</td>
<td>The numerical results did not provide consistent quantitative results for the transient variation of total water input, transient temperature change, relative humidity and total stresses&lt;br&gt;Good correlation was achieved between the experimentally measured and numerically simulated results. (Alonso and Alcoverro, 1999) (cont’d)</td>
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A series of thermal-hydraulic experiments on a bentonite buffer compacted in a borehole and surrounded by a granite block are described as follows:

- A sealed interface was used to prevent moisture migration from the buffer to the granite and moisture loss to the atmosphere.
- The interface had an a thin highly permeable liner which was kept saturated at all times.
- The buffer was placed in direct contact with a dry porous rock mass where the water would migrate from the buffer to the rock.

Selvadurai (1996) concluded from the analysis of the three aforementioned experiments that the moisture losses were primarily induced by the heat conduction process, resulting in impedance to the heat transfer within the experiment.

In the second experiment a substantial increase in the moisture content of the buffer and swelling was observed.

Selvadurai (1996) believed that moisture adsorption and retention within the buffer had a positive impact on the heat transfer from the source to the host rock. He added that an accelerated uptake of moisture into buffer is good for the transfer of heat from the waste canister to the rock, and for maintaining a defect free buffer.

| Power, Reactor and Nuclear Fuel Development Corporation (PNC) (layout refer to figure 2.8) | A full-scale thermo/hydro/mechanical coupled test based on a pit disposal concept. | Kanno et al., (1999) found that the numerical results’ temperature profiles were approximately 5 Celsius lower than the measured results. However good correlation was achieved. |

| McGill University, Canada (layout refer to figure 2.7) | A series of thermal-hydraulic experiments on a bentonite buffer compacted in a borehole and surrounded by a granite block are described as follows: - A sealed interface was used to prevent moisture migration from the buffer to the granite and moisture loss to the atmosphere. The interface had an a thin highly permeable liner which was kept saturated at all times. The buffer was placed in direct contact with a dry porous rock mass where the water would migrate from the buffer to the rock. | Selvadurai (1996) concluded from the analysis of the three aforementioned experiments that the moisture losses were primarily induced by the heat conduction process, resulting in impedance to the heat transfer within the experiment. |

Table 2.1  A summary on large scale mock-up experiments performed by various institutions
a) A single silica tetrahedron unit

b) A single octahedral unit

Figure 2.1 Sketches of a tetrahedral and an octahedral unit (Scott, 1994)
Stacking of n unit layers forming single particle. Hydration in interlayers occupy interlayer pores.

Representative Elementary
Volume REV

Cluster of particles, tactoids and single unit layers. Pore spaces identified as micropores.

Single 2:1 unit layer acting as single particle, e.g. Na-montmorillonite

Hierarchy of fabric units
- single unit layers
- particles (stacking of 'n' unit layers)
- domains or tactoids ('n' number of particles)
- clusters (mixed grouping of particles, domains/tactoids)
- ped (aggregation of particles, domains and clusters)

Figure 2.2 Hierarchical Order of Fabric Units and Pore Spaces (Yong, 1999)
Figure 2.3 Diffusivity and viscosity of the external water [extracted from Ichikawa (1999)]
Figure 2.4  Three-scale model for Clay [extracted from Murad and Cushman (1997)]
Figure 2.5  Full-scale model of an engineered barrier made of a compacted swelling clay, (Felix et al, 1996)
Figure 2.6  The FEBEX mock-up test assembly showing its main components; the confining structure, the two heaters (in black) and the clay barrier, (Catsius Clay, 1999)
Figure 2.7 The granite block test facility, (Selvadurai, 1996)
Figure 2.8  Schematic of the BIG-BEN facility, (Kanno et al., 1999)
Figure 2.9  Location, orientation and codes of the sensors on the BACCHUS 2 experiment, (Volckaert et al., EUR 16860, 1996)
Figure 2.10  CERBERUS – Lay-out of the test
Chapter 3

Theoretical Formulation

3.1 Introduction

This chapter presents the theoretical formulation for thermal/hydraulic/mechanical behaviour of unsaturated soils. The formulation shown in this chapter has been presented previously and does not form part of the author’s contribution. However it is necessary to repeat this here so that readers can have a better understanding of the formulations used in the numerical model.

The governing equations are expressed in terms of four primary variables: pore water pressure ($u_t$), pore air pressure ($u_a$), temperature ($T$), and displacement ($u$).

In Section 3.2 the law of conservation of mass is applied to describe the governing equation for moisture flow. As the flow of moisture is governed by liquid and vapour effects, both have been considered in this chapter.

In Section 3.3 the law of mass conservation is again used to produce the governing equation for air flow. As the air phase is considered a binary mixture of dry air and water vapour, the governing equation has accounted for effects from both cases.

Section 3.4 presents the governing equation for heat transfer. The conduction, convection and/or latent heat of vaporisation have all been considered in the derivation of the heat transfer governing equation.
Section 3.5 presents the stress-strain behaviour of unsaturated soil modelled using an 
elasto-plastic work hardening constitutive model. The governing equation for 
deformation is derived from considerations of stress equilibrium.

And finally in Section 3.6 a summary of the governing equations which describe flow 
and deformation is presented.

3.2 Theoretical development of the governing equation for moisture transfer

Moisture transfer in unsaturated soil may be considered as a two phase flow; the flow 
of liquid water and the flow of water vapour. The following equation defines the sum 
of the volumetric water content, \( \theta \), as the sum of these two phases;

\[
\theta = \theta_l + \theta_v
\]  
(3.1)

where \( \theta_l \) is the volumetric liquid content and \( \theta_v \) is the volumetric vapour content.

Both liquid and vapour phases can be considered separately before applying the law 
of mass conservation on moisture. The principle of thermodynamic equilibrium 
dictates that at any point, the volumetric liquid water and water vapour are in 
equilibrium (de Vries, 1958) giving;

\[
\theta_v = \frac{(n - \theta_l) \rho_v}{\rho_l}
\]  
(3.2)

where, \( n \) is the porosity, \( \rho_v \) is the density of water vapour and \( \rho_l \) is the density of 
liquid water.

For the liquid water phase, the law of conservation of mass dictates that the time 
derivative of the liquid content is equal to the gradient of the liquid flux. This can be 
expressed as;

\[
\rho_l \frac{\partial \theta_l}{\partial t} \nabla = -\rho_l \nabla \nabla \cdot \mathbf{v}_l - \rho_l \nabla E_{ss}
\]  
(3.3)

where \( t \) is time, \( \mathbf{v}_l \) is the velocity of liquid, \( E_{ss} \) is a sink/source term, \( \nabla \) is the gradient 
operator and \( \nabla \) is the incremental volume.
Similarly for the vapour phase, the law of conservation of mass dictates that the time derivative of the vapour content is equal to the gradient of the vapour flux. This can be expressed mathematically as:

$$\rho_v \frac{\partial \theta_v \partial V}{\partial t} = -\rho_i \partial V \nabla \cdot \vec{v}_v - \partial V \nabla \left( \rho_v \vec{v}_v \right) + \rho_i \partial V E_{ss}$$

(3.4)

where $\vec{v}_v$ is the velocity of vapour and $\vec{v}_a$ is the velocity of pore air. The volumetric air content, $\theta_a$, can be expressed as:

$$\theta_a = (n - \theta_l)$$

(3.5)

Substituting Equations (3.2) and (3.5) into Equation (3.4), the law of mass conservation for liquid vapour flow is now expressed in terms of porosity and volumetric air content;

$$\rho_i \frac{\partial \theta_\ell \partial V}{\partial t} = -\rho_i \partial V \nabla \cdot \vec{v}_\ell - \partial V \nabla \left( \rho_i \vec{v}_\ell \right) + \rho_i \partial V E_{ss}$$

(3.6)

Combining the equations for liquid and vapour flow in Equation 3.3 and 3.6 respectively, the mass conservation equation for moisture flow is given as;

$$\rho_i \frac{\partial \theta_\ell \partial V}{\partial t} + \rho_i \frac{\partial \theta_a \partial V}{\partial t} = -\rho_i \partial V \nabla \cdot \vec{v}_\ell - \partial V \nabla \left( \rho_i \vec{v}_\ell \right) - \partial V \nabla \left( \rho_i \vec{v}_a \right)$$

(3.7)

The volumetric liquid and air contents can also be expressed in terms of porosity and degree of saturation, which gives the following;

$$\theta_\ell = n S_\ell$$

(3.8)

$$\theta_a = n S_a$$

(3.9)

where $S_\ell$ is the degree of saturation of pore water and $S_a$ is the degree of saturation of pore air.

The volume increment, $\partial V$ is the summation of the void volume and solid volume. This can also be represented as;

$$\partial V = (1 + e) \partial V_s$$

(3.10)
Chapter 3 Theoretical Formulation

where $V_s$ is the volume of the solids.

Substituting equations (3.8), (3.9) and (3.10) into equation (3.7), gives;

$$\rho_i \frac{\partial (nS_t (1 + e) \partial V_s)}{\partial \alpha} + \rho_i \frac{\partial (\rho_e S_s (1 + e) \partial V_s)}{\partial \alpha} + \rho_i (1 + e) \partial V_s \nabla V_1 + \rho_i (1 + e) \partial V_s \nabla (\rho, v) = 0$$

(3.11)

Since soil is assumed as incompressible, the volume of soil would remain constant and the term $\partial V_s$ can be eliminated from Equation (3.11). The porosity, $n$ can also be represented by $(1+e)e$. Therefore incorporating both changes to Equation (3.11) gives;

$$\rho_i \frac{\partial (nS_t)}{\partial \alpha} + \rho_i \frac{\partial (\rho S_s n)}{\partial \alpha} + \rho_i \nabla V_1 + \rho_i \nabla V_v + \nabla (\rho, v) = 0$$

(3.12)

Inspection of the spatial derivatives terms of Equation (3.12) reveals that the moisture flux constitutes a liquid flux term; a component of vapour flux due to vapour pressure gradients; and a component of vapour flux arising from the bulk flow of vapour due to movement of pore air. In addition, the equation shows the movement of water is governed by the velocities of the liquid, vapour and air phases. These flow rates and the flow laws that govern them are discussed below.

3.2.1 Mechanisms of liquid flow

In this study, the flow of water is considered to be caused by pressure head, elevation head and thermal gradients (Mitchell, 1993). The flow of liquid water due to electrical gradients is not considered.

The first two of these mechanisms; pressure head, and elevation head, may be combined to give the hydraulic head gradient. This is considered to be a driving potential for water flow. These mechanisms have been described by Darcy’s law (1856), and this approach has been applied to unsaturated soil by Childs, (1969). For multiphase flow in unsaturated soil, Darcy’s law may be expressed as;

$$v_1 = -\frac{K_l}{\mu_l} \left[ \nabla \left( \frac{u_l}{\gamma_l} \right) + \nabla z \right] = -k_i \left[ \nabla \left( \frac{u_l}{\gamma_i} \right) + \nabla z \right] \text{ (m/s)}$$

(3.13)
where \( v_i \) is the liquid velocity due to pressure and elevation heads, \( K_i \) is the effective permeability, \( \mu_i \) is the absolute viscosity of pore liquid, \( k_i \) is the unsaturated hydraulic conductivity, \( \gamma_i \) is the unit weight of liquid and \( z \) is the elevation.

The absolute viscosity of the liquid water is temperature dependent. A relationship between the dynamic viscosity of the liquid water and the absolute temperature was presented by Kaye and Laby, (1973);

\[
\mu_i(T) = 661.2(T - 229)^{-1.562} \times 10^{-3} + 0.5\% (\text{Ns/m}^2) \tag{3.14}
\]

Researchers have found that the unsaturated hydraulic conductivity may be defined by two of three possible mass volume properties; void ratio, \( e \), degree of liquid saturation, \( S_i \), or volumetric water content, \( \theta_i \) (Lloret and Alonso, 1980; Fredlund, 1991). In this formulation, void ratio and degree of liquid saturation have been adopted;

\[
k_i = k_i(e, S_i) \quad (\text{m/s}) \tag{3.15}
\]

Matyas and Radhakrishna, (1968) proposed that the degree of liquid saturation is a function of the initial void ratio, the initial degree of liquid saturation, and the stress parameters, namely; net stress, deviatoric stress, and suction. However, Alonso et al., (1988) found the influence of stress on the degree of saturation to be relatively insignificant. Therefore if the initial conditions of a soil sample are controlled, the degree of saturation can be expressed as a function of soil suction, \( s \);

\[
S_i = S_i(s) \tag{3.16}
\]

In this formulation, the soil suction has been expressed as the free energy state of soil water. Adopting the relationship established by Edelfsen and Anderson (1943) which relates the surface energy, \( \xi \), as a function of temperature;

\[
\xi = 0.1171 - 0.00015167 T \quad (\text{J/m}^2) \tag{3.17}
\]

Therefore the suction at any degree of liquid saturation and temperature can be given provided a relationship between suction and degree of saturation, and a reference temperature, \( T_r \), are known;
where \( s_r \) and \( \xi_r \) are the suction and the surface energy at the reference temperature \( T_r \), and \( s \) and \( \xi \) are the suction and the surface energy at the actual temperature \( T \).

If the dependence of soil suction on temperature is incorporated into Equation (3.16) the degree of saturation may be expressed in partial derivative form as:

\[
\frac{\partial S_i}{\partial t} = \frac{\partial S_i}{\partial s} \frac{\partial s}{\partial t} + \frac{\partial S_i}{\partial T} \frac{\partial T}{\partial t}
\]  

(3.19)

Matric suction is defined as the difference between pore air pressure and pore liquid pressure, and is mathematically expressed as, (Fredlund and Rahardjo, 1993);

\[
s = u_a - u_l
\]  

(Pa)  

(3.20)

Substituting Equation (3.20) into Equation (3.19), the degree of saturation relationship may be expressed as;

\[
\frac{\partial S_i}{\partial t} = \frac{\partial S_i}{\partial s} \frac{\partial u_a}{\partial t} + \frac{\partial S_i}{\partial T} \frac{\partial T}{\partial t} - \frac{\partial S_i}{\partial s} \frac{\partial u_l}{\partial t}
\]  

(3.21)

3.2.2 **Mechanisms of vapour flow**

Vapour transfer occurs as a result of two main mechanisms, namely; diffusive and pressure flows. The bulk air is considered to be a binary mixture of water vapour and dry air (Pollock, 1986) and is described using a generalised Darcy’s law. Diffusive vapour flow in unsaturated soil has been described by Philip and de Vries (1957). Pressure gradient is considered as the only driving potential as the elevation gradient is considered to have a negligible effect for small scale problems (Fredlund and Rahardjo, 1993). As such, a generalised Darcy’s law for multiphase flow in unsaturated soil can be defined as;

\[
v_a = -\frac{K_a}{\mu_a} \nabla u_a = -k_a \nabla u_a
\]  

(m/s)  

(3.22)
\( v_a \) is the velocity of pore air, \( K_a \) is the effective permeability of pore air, \( \mu_a \) is the absolute viscosity of pore air, \( u_a \) is the pore air pressure and \( k_a \) is the unsaturated conductivity of pore air.

The unsaturated conductivity of gases in soil is a function of the fluid and soil volume/mass properties. As the fluid properties are generally assumed to be constant during the flow process, the volume/mass properties effectively controls the air conductivity, (Olson, 1963). In this study the volume/mass properties chosen are void ratio and degree of pore air saturation;

\[
k_a = k_a(e, S_a)
\]

(3.23)

The Philip and de Vries (1957) approach with an extension by Ewen and Thomas (1989) are applied to describe the diffusive flow contribution to vapour transport. Using this approach, the velocity of vapour, \( v_v \) through an unsaturated soil is defined as;

\[
v_v = -\frac{D_{atms} v_v \tau_v \theta_a}{\rho_v} \nabla \rho_v \quad \text{(m/s)}
\]

(3.24)

where \( D_{atms} \) is the molecular diffusivity of vapour through air, \( \tau_v \) is the tortuosity factor, \( v_v \) is a mass flow factor and \( \nabla \rho_v \) is the vapour density gradient.

The molecular diffusivity may be based on an approach adopted by Philip and de Vries, (1957). They have included a relationship proposed by Krischer and Rohnalter, (1940) for molecular diffusivity due to a temperature gradient. This is shown as;

\[
D_{atms} = 5.893 \times 10^{-6} \frac{T^{2.3}}{\mu_a} \quad \text{(m}^2/\text{s)}
\]

(3.25)

Phillip and de Vries, (1957) introduced an expression for the mass flow factor \( v_v \). It was incorporated to ‘allow for the mass flow of vapour arising from the difference in boundary conditions governing the air and vapour components of the diffusion system’. The expression proposed by Partington and de Vries, (1957) was adopted,
who showed that for steady state diffusion in a closed system between an evaporating source and a condensing sink;

\[ \nu_v = \frac{u_e - u_v}{u_a - u_v} \]  

(3.26)

where \( u_v \) is the partial pressure of vapour and can be calculated as;

\[ u_v = \rho_v R_v T \]  

(Pa)  

(3.27)

where \( R_v \) is the specific gas constant for water vapour (461.5 J/KgK). It was recognised by Philip and de Vries (1957) that the predicted value of the mass flow factor, \( \nu_v \), from equation (3.26) may not be valid for non-stationary conditions, but the expression was able to predict the correct order of magnitude. They also remarked that the factor is close to 1 at normal soil temperatures.

Using the thermodynamic relationship proposed by Edlefsen and Anderson (1943) the density of water vapour \( \rho_v \) can be represented by;

\[ \rho_v = \rho_0 h = \rho_0 \exp \left( \frac{\psi g}{R_v T} \right) \]  

(kg/m³)  

(3.28)

where \( \rho_0 \) is the density of saturated water vapour, \( h \) is the relative humidity, \( g \) is the gravitational constant and \( \psi \) is the capillary potential which is defined as;

\[ \psi = \frac{u_i - u_a}{\gamma_i} \]  

(m)  

(3.29)

Ewen and Thomas (1989) presented a relationship to fit into the standard data (Mayhew and Rogers, 1976) for the density of saturated water vapour;

\[ \rho_0 = 10^{\left\lfloor 94.4 \exp \left( -0.06374 \left( T - 273 \right) + 0.1634 \times 10^{-3} \left( T - 273 \right)^2 \right) \right\rfloor} \]  

(3.30)

From Equation (3.28) it can be observed that the density of water vapour \( \rho_v \), is dependent on the saturated soil water vapour, \( \rho_0 \), and the relative humidity, \( h \). As \( \rho_0 \) is dependent on the absolute temperature, \( T \), and the relative humidity is dependent on both suction and temperature; the gradient of vapour density may be expressed as;
\[ \nabla \rho_v = h \nabla \rho_0 + \rho_0 \nabla h \] (3.31)

Equation (3.31) can be expanded to give;

\[ \nabla \rho_v = \left( h \frac{\partial \rho_0}{\partial T} \right) \nabla T + \rho_0 \left( \frac{\partial \mathcal{H}}{\partial s} \cdot \nabla s + \frac{\partial \mathcal{H}}{\partial T} \cdot \nabla T \right) \] (3.32)

Including equation (3.20) for suction and rearranging the terms yields;

\[ \nabla \rho_v = \left( h \frac{\partial \rho_0}{\partial T} + \rho_0 \frac{\partial \mathcal{H}}{\partial T} \right) \nabla T + \left( \rho_0 \frac{\partial \mathcal{H}}{\partial s} \right) \nabla u_a - \left( \rho_0 \frac{\partial \mathcal{H}}{\partial s} \right) \nabla u_i \] (3.33)

Also the time derivative can be shown to yield;

\[ \frac{\partial \rho_v}{\partial t} = \left( h \frac{\partial \rho_0}{\partial T} + \rho_0 \frac{\partial \mathcal{H}}{\partial T} \right) \frac{\partial T}{\partial \alpha} + \left( \rho_0 \frac{\partial \mathcal{H}}{\partial s} \right) \frac{\partial u_a}{\partial \alpha} - \left( \rho_0 \frac{\partial \mathcal{H}}{\partial s} \right) \frac{\partial u_i}{\partial \alpha} \] (3.34)

Substituting equation (3.33) into equation (3.24) yields;

\[ v_v = \frac{D_{ams} v_s \tau_s \theta_a}{\rho_i} \left( \rho_0 \frac{\partial \mathcal{H}}{\partial s} \right) \nabla u_i - \frac{D_{ams} v_s \tau_s \theta_a}{\rho_i} \left( h \frac{\partial \rho_0}{\partial T} + \rho_0 \frac{\partial \mathcal{H}}{\partial T} \right) \nabla T \]

\[- \frac{D_{ams} v_s \tau_s \theta_a}{\rho_i} \left( \rho_0 \frac{\partial \mathcal{H}}{\partial s} \right) \nabla u_a \] (3.35)

Experimental work carried out by Philip and de Vries (1957) suggested that the simple theory defined in Equation (3.35) was not entirely accurate at increased temperature gradients. Two refinements were made to the thermal gradient term. Firstly a flow area factor, \( f \), was included to achieve a reduction of the vapour flow as the available flow area decreased at higher moisture contents. Secondly a microscopic pore temperature gradient factor, \( (\nabla T)_a/(\nabla T) \), was introduced, which is the ratio of the average temperature gradient in the air filled pores to the overall temperature gradient. This factor takes account of the microscopic effect of heat flow paths being shared between sections of solid and fluid paths, giving rise to microscopic temperature gradients in the fluid filled pores, which may be much higher than the macroscopic temperature gradients across the sample as a whole. Including these two amendments into equation (3.35) yields;
\[ v_x = \frac{D_{\text{awm}} v_n}{\rho_l} \left( \frac{\partial \tilde{h}}{\partial \tilde{c}} \right) \nabla u_x - \frac{f D_{\text{awm}} v_n}{\rho_l} \frac{(\nabla T)_n}{\nabla T} \left( h \frac{\partial \rho_o}{\partial T} + \rho_o \frac{\partial \tilde{h}}{\partial T} \right) \nabla T - \frac{D_{\text{awm}} v_n}{\rho_l} \left( \frac{\partial \tilde{h}}{\partial \tilde{c}} \right) \nabla u_a \]  

(3.36)

de Vries (1966) adopted a proposal by Preece (1975) who presented an expression to evaluate the microscopic pore temperature gradient factor, \((\nabla T)_o / (\nabla T)\), based on a proposed geometrical method. The expression was developed for a Washington Sand, and is adopted here as experimental evidence was lacking to develop the approach for fine grained soils.

\[ \frac{(\nabla T)_o}{\nabla T} = \frac{1}{3} \left[ \frac{2}{1 + B G_v} + \frac{1}{1 + B(1 - 2 G_v)} \right] \]  

(3.37)

where,

\[ B = \frac{(\lambda_a + \lambda_v)}{\lambda_l} - 1 \]  

(3.38)

and,

\[ G_v = \begin{cases} 
0.3333 - 0.325(n - \theta)/n & 0.09 < \theta_l < n \\
0.0033 + 11.1(0.33 - 0.325(n - 0.09)/n)\theta_l & 0 < \theta_l < 0.09 
\end{cases} \]  

(3.39)

\( \lambda_a \) is the thermal conductivity of pore air, \( \lambda_l \) is the thermal conductivity of pore liquid and \( \lambda_v \) is the thermal conductivity of pore vapour, which can be defined as;

\[ \lambda_l = D_{\text{awm}} v_n h L \frac{\partial \rho_o}{\partial T} \]  

(3.40)

where \( L \) is the latent heat of vaporisation.

### 3.2.3 Governing differential equation for water flow

Having defined and presented the components of flow for the liquid and vapour phases, Equation (3.12) may be rewritten to give the governing differential equations for moisture flow. Before that, some terms needs to be further developed and have been detailed here.
Expanding the first two terms of the equation (3.12) and noting that \( S_a = 1 - S_t \), leads to the following expression:

\[
e(\rho_t - \rho_v) \frac{\partial S_i}{\partial t} + e(1 - S_t) \frac{\partial \rho_v}{\partial t} + \left[ \rho_t S_i + \rho_v (1 - S_t) \right] \frac{\partial e}{\partial t} + \\
\rho_t (1 + e) \nabla \cdot \mathbf{v}_1 + \rho_v (1 + e) \nabla \cdot \mathbf{v}_v + (1 + e) \nabla \cdot (\rho_v v_v) = 0
\]  

(3.41)

Dividing equation (3.41) by \((1 + e)\) and replacing \( e/(1+e) \) by \( n \) yields:

\[
n(\rho_t - \rho_v) \frac{\partial S_i}{\partial t} + n(1 - S_t) \frac{\partial \rho_v}{\partial t} + \left[ \rho_t S_i + \rho_v (1 - S_t) \right] \frac{\partial e}{\partial t} + \\
\rho_t \nabla \cdot \mathbf{v}_1 + \rho_v \nabla \cdot \mathbf{v}_v + \nabla \cdot (\rho_v v_v) = 0
\]  

(3.42)

Considering the third term, it can be shown that:

\[
\frac{\partial e}{(1 + e) \partial t} = \frac{\partial \varepsilon_v}{\partial t}
\]  

(3.43)

where \( \varepsilon_v \) is the volumetric strain which by definition is the rate of change of void ratio with respect to initial volume. Substituting this term into Equation (3.42) gives:

\[
n(\rho_t - \rho_v) \dot{\varepsilon}_v + n(1 - S_t) \frac{\partial \rho_v}{\partial t} + \left[ \rho_t S_i + \rho_v (1 - S_t) \right] \frac{\partial \varepsilon_v}{\partial t} + \\
\rho_t \nabla \cdot \mathbf{v}_1 + \rho_v \nabla \cdot \mathbf{v}_v + \nabla \cdot (\rho_v v_v) = 0
\]  

(3.44)

The first term of Equation (3.44) can be expressed, with appropriate substitution from equation (3.21), as:

\[
n(\rho_t - \rho_v) \frac{\partial S_i}{\partial t} = -n(\rho_t - \rho_v) \frac{\partial \varepsilon_l}{\partial t} \frac{\partial u_l}{\partial t} + n(\rho_t - \rho_v) \frac{\partial S_i}{\partial t} \frac{\partial \varepsilon_T}{\partial \varepsilon_T} + \\
+ n(\rho_t - \rho_v) \frac{\partial S_i}{\partial \varepsilon} \frac{\partial u_v}{\partial \varepsilon}
\]  

(3.45)

With substitution from equation (3.34) the second term can be expressed as:

\[
n(1 - S_t) \frac{\partial \rho_v}{\partial t} = \\
n(1 - S_t) \left[ \left( \frac{\partial h}{\partial t} + \rho_0 \frac{\partial h}{\partial \varepsilon} \right) \frac{\partial \varepsilon_T}{\partial \varepsilon} + \left( \rho_0 \frac{\partial H}{\partial \varepsilon} \right) \frac{\partial u_v}{\partial \varepsilon} - \left( \rho_0 \frac{\partial H}{\partial \varepsilon} \right) \frac{\partial u_l}{\partial \varepsilon} \right]
\]  

(3.46)
Chapter 3

Theoretical Formulation

It can be shown that:

\[
\frac{\partial \varepsilon_v}{\partial t} = (1 + e) \frac{\partial n}{\partial t} = m^T \frac{\partial \varepsilon_v}{\partial t} = m^T P \frac{\partial u}{\partial t}
\]  

(3.47)

where \( \varepsilon_v \) is the volumetric strain and \( \varepsilon \) is the strain vector. The strain matrix \( P \) and the differential operator \( m \) will be defined in Section 3.6. The third term of equation (3.44) can therefore be expressed as:

\[
\left( \rho_i S_i + \rho_v (1 - S_i) \right) \frac{\partial \varepsilon_v}{\partial t} = \left( \rho_i S_i + \rho_v (1 - S_i) \right) m^T P \frac{\partial u}{\partial t}
\]  

(3.48)

Substituting equations (3.45), (3.46) and (3.48) for the first, second and third terms respectively and equations (3.13), (3.22) and (3.36) for \( v_i, v_a \) and \( v_r \) respectively into Equation (3.44) yields the governing differential equation for water transfer in terms of the primary variables:

\[
C_{ii} \frac{\partial u_i}{\partial t} + C_{ir} \frac{\partial T}{\partial t} + C_{iiu} \frac{\partial u_a}{\partial t} + C_{iu} \frac{\partial u_r}{\partial t} = \\
\nabla \left[ K_{ii} \nabla u_i \right] + \nabla \left[ K_{ir} \nabla T \right] + \nabla \left[ K_{ia} \nabla u_a \right] + \nabla \sum_{j=1}^{N} \rho_l K_{l_j} \nabla c_{l_j} + J_i
\]  

(3.49)

where

\[
C_{ii} = -n(\rho_i - \rho_v) \frac{\partial S_i}{\partial s} - n(1 - S_i) \rho_0 \frac{\partial h}{\partial s}
\]  

(3.50)

\[
C_{ir} = n(\rho_i - \rho_v) \frac{\partial S_i}{\partial T} + n(1 - S_i) \left( h \frac{\partial \rho_0}{\partial T} + \rho_0 \frac{\partial h}{\partial T} \right)
\]  

(3.51)

\[
C_{ia} = n(\rho_i - \rho_v) \frac{\partial S_i}{\partial s} + n(1 - S_i) \rho_0 \frac{\partial h}{\partial s}
\]  

(3.52)

\[
C_{iu} = (S_i \rho_i + (1 - S_i) \rho_v) m^T P
\]  

(3.53)

\[
K_{ii} = \rho_i \left[ \frac{k_i}{\gamma_i} - \frac{D_{amps} v_a n}{\rho_i} \left( \rho_0 \frac{\partial h}{\partial s} \right) \right]
\]  

(3.54)
\[ K_{\text{fr}} = \rho_i \frac{D_{\text{ann}} M T}{\rho_i \nabla T} \left( h \frac{\partial p_0}{\partial T} + p_0 \frac{\partial h}{\partial T} \right) \]  
\[ (3.55) \]

\[ K_{\text{ia}} = \rho_i k_a + \rho_i \left[ \frac{D_{\text{ann}} M T}{\rho_i} \left( p_0 \frac{\partial h}{\partial s} \right) \right] \]  
\[ (3.56) \]

\[ J_i = \rho_i \nabla (K_i \nabla z) \]  
\[ (3.57) \]

### 3.3 Dry air transfer

Dry air transfer in unsaturated soil is believed to be driven by bulk air and dissolved air flow (Rodebush and Busswell, 1958). The bulk air transfer occurs when there is a gradient of air pressure. The dissolved air is transferred within the pore liquid itself. Bulk air transfer is determined via Darcy's Law, and the volume of dry air within the pore liquid is determined via Henry's Law.

Applying the law of conservation of mass the temporal derivative of the dry air content is equal to the spatial derivative of the dry air flux. Mathematically this can be expressed as;

\[ \frac{\partial}{\partial \alpha} \left[ \theta_s + H_s \theta_i \right] \rho_{\text{da}} \frac{\partial V}{\partial \alpha} = -\nabla \cdot \left[ \rho_{\text{da}} \left( \mathbf{v}_s + H_s \mathbf{v}_1 \right) \right] \]  
\[ (3.58) \]

where \( H_s \) is Henry's volumetric coefficient of solubility and \( \rho_{\text{da}} \) is the density of dry air.

Substituting Equations (3.8), (3.9) and (3.10) into Equation (3.58) yields;

\[ \frac{\partial}{\partial \alpha} \left[ S_s + H_s S_i \right] n \rho_{\text{da}} \left( 1 + e \right) \frac{\partial V}{\partial \alpha} = -\left( 1 + e \right) \nabla \cdot \left[ \rho_{\text{da}} \left( \mathbf{v}_s + H_s \mathbf{v}_1 \right) \right] \]  
\[ (3.59) \]

Eliminating the term \( \partial V \) and substituting \( n(1 + e) = e \) and \( S_s = 1 - S_i \) gives;

\[ \frac{\partial}{\partial \alpha} \left[ (1 - S_i + H_s S_i) \rho_{\text{da}} e \right] + (1 + e) \nabla \left[ \rho_{\text{da}} \left( \mathbf{v}_s + H_s \mathbf{v}_1 \right) \right] = 0 \]  
\[ (3.60) \]

Expanding the first term of (3.60) and rearranging similar terms gives;
Rearranging similar terms yields;

\[
\frac{\partial}{\partial t}[1 - S_i + H_s S_i] \rho_{da} e = \rho_{da} (1 - S_i + H_s S_i) \frac{\partial e}{\partial t} + e(1 - S_i + H_s S_i) \frac{\partial \rho_{da}}{\partial t} + e \rho_{da} (H_s - 1) \frac{\partial S_i}{\partial t} \tag{3.61}
\]

Substituting Equation (3.61) into (3.60) and dividing the resultant equation by (1+e) whilst replacing \(e/(1+e)\) by \(n\) yields;

\[
\rho_{da} \left( \frac{1 - S_i + H_s S_i}{1+e} \right) \frac{\partial e}{\partial t} + n(1 - S_i + H_s S_i) \frac{\partial \rho_{da}}{\partial t} + n \rho_{da} (H_s - 1) \frac{\partial S_i}{\partial t} + \nabla [\rho_{da} (v_s + H_s v)] = 0 \tag{3.62}
\]

Substituting equations (3.43) and (3.47) into (3.62) yields;

\[
\rho_{da} \left( 1 - S_i + H_s S_i \right) m^t P \frac{\partial u}{\partial t} + n(1 - S_i + H_s S_i) \frac{\partial \rho_{da}}{\partial t} + n \rho_{da} (H_s - 1) \frac{\partial S_i}{\partial t} + \nabla [\rho_{da} (v_s + H_s v)] = 0 \tag{3.63}
\]

The air phase in soils has been found to obey the laws of a mixture of ideal gases to a sufficient degree of accuracy (Geraminegad and Saxena, 1986). Therefore the partial pressures of dry air and vapour can be expressed as;

\[
\begin{align*}
    u_{da} &= \rho_{da} R_{da} T \quad \text{(Pa)} \tag{3.64} \\
    u_v &= \rho_v R_v T \quad \text{(Pa)} \tag{3.65}
\end{align*}
\]

where \(R_v\) and \(R_{da}\) represent the specific gas constants of vapour and dry air respectively.

To determine the dry air density, the combination of Equations (3.64) and (3.65) gives:

\[
\rho_{da} = \frac{u_a}{R_{da} T} - \frac{\rho_v R_v}{R_{da}} \quad \text{(kg/m}^3\text{)} \tag{3.66}
\]

The partial derivative of equation (3.66) with respect to time can be expressed as follows, wherein the last differential term can be obtained from equation (3.34);
\[
\frac{\partial \rho_i}{\partial t} = \frac{1}{R_{da} T} \frac{\partial \rho_i}{\partial t} + \frac{\rho_a}{T} \frac{\partial T}{\partial t} - \frac{R_v}{R_{da}} \frac{\partial \rho_v}{\partial t} \quad (3.67)
\]

Substituting for the terms \( \frac{\partial S_i}{\partial t} \), \( \frac{\partial \rho_{da}}{\partial t} \), \( v_i \) and \( v_a \) from equations (3.19), (3.67), (3.13) and (3.22) respectively leads to the governing equation;

\[
C_{al} \frac{\partial u_i}{\partial t} + C_{aT} \frac{\partial T}{\partial t} + C_{aa} \frac{\partial u_a}{\partial t} + C_{au} \frac{\partial u}{\partial t} = \\
\nabla [K_{al} \nabla u_i] + \nabla [K_{aa} \nabla u_a] + \nabla [K_{ai} \nabla c_i] + J_a \quad (3.68)
\]

where;

\[
C_{al} = -n \rho_{da} (H_i - 1) \frac{\partial S_i}{\partial t} + n (S_a + H_i S_i) \frac{R_v}{R_{da}} \left( \rho_o \frac{\partial H}{\partial t} \right) \quad (3.69)
\]

\[
C_{aT} = n \rho_{da} (H_i - 1) \frac{\partial S_i}{\partial t} - n (S_a + H_i S_i) \left( \frac{\rho_a}{T} - \frac{R_v}{R_{da}} \left( h \frac{\partial \rho_0}{\partial T} + \rho_0 \frac{\partial H}{\partial T} \right) \right) \quad (3.70)
\]

\[
C_{aa} = n \rho_{da} (H_i - 1) \frac{\partial S_i}{\partial t} + n (S_a + H_i S_i) \left( \frac{1}{R_{da} T} - \frac{R_v}{R_{da}} \rho_o \frac{\partial H}{\partial t} \right) \quad (3.71)
\]

\[
C_{au} = \rho_{da} (S_a + H_i S_i) m^T P \quad (3.72)
\]

\[
K_{al} = \frac{\rho_{da} H_i}{\gamma_i} k_i \quad (3.73)
\]

\[
K_{aa} = \rho_{da} k_a \quad (3.74)
\]

\[
J_a = \rho_{da} H_i \nabla \left( k_i \nabla z \right) \quad (3.75)
\]

### 3.4 Heat transfer

Three principal methods of heat transfer have been identified: conduction, convection, and radiation (Jakob, 1949). The effect of heat radiation is ignored as its influence is assumed to be negligible. The effect of latent heat of vaporisation is however included.
Chapter 3  

Theoretical Formulation

The law of conservation of energy for heat flow dictates that the temporal derivative of the heat content \( \Omega \), is equal to the spatial derivative of the heat flux, \( \mathbf{Q} \). This may be expressed as:

\[
\frac{\partial (\Omega \partial V)}{\partial t} = -\nabla \mathbf{Q} \cdot (\partial V)
\]  

(3.76)

The heat content of unsaturated soil per unit volume, \( \Omega \), is assumed to be the sum of soil heat storage capacity and the contribution resulting from the latent heat of vaporisation. This can be defined as:

\[
\Omega = H_c(T - T_r) + L \rho_v
\]  

(3.77)  

where \( L \) represents the latent heat of vaporisation.

Following the approach presented by Ewen and Thomas (1989), the heat capacity of unsaturated soil, \( H_c \), at reference temperature, \( T_r \), may be defined as:

\[
H_c = (1 - n)C_{ps} \rho_s + n\left( C_{pl} S_p \rho_l + C_{pv} S_a \rho_v + C_{pda} S_a \rho_{da} \right)
\]  

(J/m\(^3\))  

(3.78)

where \( C_{ps}, C_{pl}, C_{pv}, \) and \( C_{pda} \) are the specific heat capacities of solid particles, liquid, vapour, and dry air respectively and \( \rho_s \) is the density of solid particles.

The heat flux per unit area, \( \mathbf{Q} \), is determined by:

\[
\mathbf{Q} = -\lambda T \nabla T + \left( \mathbf{v}_s \rho_v + \mathbf{v}_s \rho_v \right) L \\
+ \left( C_{pl} \mathbf{v}_l \rho_l + C_{pv} \mathbf{v}_v \rho_v + C_{pda} \mathbf{v}_s \rho_{da} \right) (T - T_r)
\]  

(W/m\(^2\))  

(3.79)

where \( \lambda \) is the coefficient of thermal conductivity of unsaturated soil.

Observing Equation (3.79) the heat transfer due to; conduction, convection, and latent heat flow associated with vapour movement have been accounted for.

Convection is considered to be the flow of heat due to movement of the liquid phase; the vapour phase arising from a vapour pressure gradient and bulk flow of air; and the air phase.
Chapter 3  Theoretical Formulation

The coefficient of thermal conductivity of unsaturated soil is taken as a function of degree of saturation, thus giving:

\[ \lambda_T = \lambda_T(S_i) \]  \hspace{1cm} \text{(W/mK)} \hspace{1cm} (3.80)

Substituting Equations (3.77) and (3.79) into Equation (3.76) yields:

\[
\frac{\partial}{\partial t} [H_c (T - T_r) + LnS_a \rho_v] \partial V =
\nabla \left[ - \lambda_T \nabla T + L(v_v \rho_v + v_s \rho_s) + \right. \nabla \left. \left( C_{pl} v_i \rho_s + C_{pv} v_v \rho_v + C_{pv} v_s \rho_v + C_{pda} v_s \rho_{da} \right) (T - T_r) \right] \partial V
\]  \hspace{1cm} (3.81)

Substituting equation (3.10) into equation (3.81), and cancelling the term \( \partial V \), yields:

\[
\frac{\partial}{\partial t} [H_c (T - T_r) + LnS_a \rho_v] (1 + e) =
\nabla \left[ - \lambda_T \nabla T + L(v_v \rho_v + v_s \rho_s) + \right. \nabla \left. \left( C_{pl} v_i \rho_s + C_{pv} v_v \rho_v + C_{pv} v_s \rho_v + C_{pda} v_s \rho_{da} \right) (T - T_r) \right] (1 + e)
\]  \hspace{1cm} (3.82)

Expanding the first term of the left hand side of the equation (3.82) yields:

\[
(T - T_r) \frac{\partial}{\partial t} [H_c(1 + e)] + H_c(1 + e) \frac{\partial T}{\partial t}
\]  \hspace{1cm} (3.83)

Considering the first term of Equation (3.83) with substitution from Equation (3.78) and rearranging the terms yields:

\[
(T - T_r) \frac{\partial}{\partial t} \left[ C_{pl} \rho_s + n(-C_{ps} \rho_s + C_{ps} S_i \rho_i + C_{pv} S_v \rho_v + C_{pda} S_{da} \rho_{da}) \right] (1 + e)
\]  \hspace{1cm} (3.84)

Expanding Equation (3.84) further and substituting \( n(1+e) = e \) yields:

\[
(T - T_r) \frac{\partial}{\partial t} \left( C_{pl} \rho_s \frac{\partial e}{\partial t} + \left( -C_{ps} \rho_s + C_{ps} S_i \rho_i + C_{pv} S_v \rho_v + C_{pda} S_{da} \rho_{da} \right) \frac{\partial e}{\partial t} + 
C_{pl} \rho_s \frac{\partial S_i}{\partial t} - C_{pv} \rho_v \frac{\partial S_i}{\partial t} + C_{ps} (1 - S_i) \frac{\partial \rho_s}{\partial t}
+ C_{pda} (1 - S_{da}) \frac{\partial \rho_{da}}{\partial t} \right)
\]  \hspace{1cm} (3.85)

From equations (3.43) and (3.47), it can be shown that:
\[ \frac{\partial e}{\partial t} = (1 + e)^2 \left( \frac{\partial n}{\partial t} \right) \]  
(3.86)

Expressing \( \frac{\partial e}{\partial t} \) in equation (3.85) in terms of \( \frac{\partial n}{\partial t} \) and rearranging the like terms yields:

\[
\begin{align*}
(T - T_r) & \left[ C_{ps} \rho_s (1 + e)^2 + (1 + e)^2 \left\{ - C_{ps} \rho_s + C_{pl} S_l \rho_l + C_{pv} S_a \rho_v + C_{pda} S_a \rho_{da} \right\} \frac{\partial n}{\partial t} \right] + \\
& \left[ e \left( C_{pl} \rho_l - C_{pv} \rho_v - C_{pda} \rho_{da} \right) \frac{\partial S_l}{\partial t} + e C_{pv} (1 - S_l) \frac{\partial \rho_v}{\partial t} + e C_{pda} (1 - S_l) \frac{\partial \rho_{da}}{\partial t} \right]
\end{align*}
(3.87)

The second term of equation (3.83) is already in the reduced form. Hence, considering the second term of equation (3.81), and substituting \( n(1+e)=e \) yields:

\[ LnS_a \rho_v (1 + e) = LeS_a \rho_v \]  
(3.88)

Expanding equation (3.88) yields:

\[ L(1 - S_l) \frac{\partial \rho_v}{\partial t} - L e \rho_v \frac{\partial S_l}{\partial t} + L(1 - S_l) \rho_v \frac{\partial e}{\partial t} \]  
(3.89)

Substituting equation (3.86) into the last term of equation (3.89) and rearrangement of the like terms yields:

\[ L(1 - S_l) \frac{\partial \rho_v}{\partial t} - L e \rho_v \frac{\partial S_l}{\partial t} + L(1 - S_l) \rho_v (1 + e)^2 \frac{\partial n}{\partial t} \]  
(3.90)

Substituting Equations (3.90), (3.87) and (3.83) into Equation (3.82) yields the governing equation for heat flow as:

\[
\begin{align*}
(T - T_r) & \left[ \left( C_{ps} \rho_s (1 + e)^2 + (1 + e)^2 \left\{ - C_{ps} \rho_s + C_{pl} S_l \rho_l + C_{pv} S_a \rho_v + C_{pda} S_a \rho_{da} \right\} \frac{\partial n}{\partial t} \right] + \\
& \left[ e \left( C_{pl} \rho_l - C_{pv} \rho_v - C_{pda} \rho_{da} \right) \frac{\partial S_l}{\partial t} + e C_{pv} (1 - S_l) \frac{\partial \rho_v}{\partial t} + e C_{pda} (1 - S_l) \frac{\partial \rho_{da}}{\partial t} \right]
\end{align*}
+ H_e (1 + e) \frac{\partial T}{\partial t} = \nabla \left[ - \lambda \nabla T + L(v \rho_v + v_s \rho_s) + \\
(\rho_{pl} v \rho_l + C_{pv} v \rho_v + C_{pda} v_s \rho_s)(T - T_r) \right] (1 + e)
\]
(3.91)

Dividing equation (3.91) by \( (1+e) \) and substituting \( e/(1+e)=n \), yields:
Substituting into the left hand side of Equation (3.92) from the derivatives with respect to time of; porosity, Equation (3.47); degree of liquid saturation, Equation (3.21); vapour density, Equation (3.34); and dry air density, Equation (3.67); rearrangement of the like terms yields the left hand side of the governing equation. This can be stated in the concise form as:

\[
(T - T_r) \left[ \frac{C_p \rho_t}{1 + e} (1 + e) \frac{\partial n}{\partial t} + n C_{pv} (1 - S_t) \frac{\partial P_v}{\partial t} + n C_{pda} (1 - S_t) \frac{\partial P_{da}}{\partial t} \right] + H_c \frac{\partial T}{\partial t} = \nabla \left[ - \lambda_T \nabla T + L(\nu_v \rho_v + \nu_s \rho_s) \right] + (C_p \nu_{ti} + C_{pv} \nu_v \rho_t + C_{pv} \nu_s \rho_s + C_{pda} \nu_s \rho_{da})(T - T_r) \]

(3.92)

where;

\[
C_{it} = \left[ \frac{- (C_p \rho_t n - C_{pv} \rho_v n - C_{pda} \rho_{da} n) \frac{\partial S_t}{\partial t} - C_{pv} S_a n \left( \rho_0 \frac{\partial h}{\partial S} \right)}{C_{pda} S_a n + \frac{R_v}{R_{da}} \left( \rho_0 \frac{\partial h}{\partial S} \right)} + \frac{\partial S_t}{\partial t} \right] (T - T_r) + \frac{\partial S_t}{\partial t} + \frac{D_{ams}}{\rho_t} \left( \rho_0 \frac{\partial h}{\partial S} \right)

(3.94)

\[
C_{TT} = H_c + \left[ \frac{C_p \rho_t n - C_{pv} \rho_v n - C_{pda} \rho_{da} n}{C_{pda} S_a n \left\{ - \frac{\partial S_t}{\partial t} - \frac{R_v}{R_{da}} \left( h \frac{\partial P_0}{\partial T} + \rho_0 \frac{\partial h}{\partial T} \right) \right\}} \right] (T - T_r)
- \frac{\partial S_t}{\partial t} + \frac{D_{ams}}{\rho_t} n \left( \nabla T \right)_a \left( h \frac{\partial P_0}{\partial T} + \rho_0 \frac{\partial h}{\partial T} \right)
\]
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\[ C_{Ta} = \left[ (C_{pi} \rho_i n - C_{pi} \rho_i n - C_{pda} \rho_{da} n) \frac{\partial H}{\partial \xi} \right] + C_{pv} S_{a} n \left( \rho_0 \frac{\partial H}{\partial \xi} \right) + \left( \frac{1}{R_{da} T} \frac{R_v}{R_{da}} \left( \rho_0 \frac{\partial H}{\partial \xi} \right) \right) \]

\[ - L \ln \rho_v \frac{\partial S_{a}}{\partial \xi} - L \ln S_{a} \left( \frac{D_{aim} \nu_n}{\rho_i} \left( \rho_0 \frac{\partial H}{\partial \xi} \right) \right) \]

(3.95)

\[ C_{Ta} = \left[ \left( - C_{ps} + C_{p} S_{i} \rho_i + C_{pv} S_{a} \rho_v + C_{pda} S_{a} \rho_{da} \right) \left( T - T_v \right) \right] + LS_a \rho_v m^T \mathbf{P} \]

(3.96)

Substituting Equations (3.13), (3.22) and (3.36) into Equation (3.92), yields;

\[ \nabla \lambda_T \nabla T - \nabla (\rho_v \nu) - \nabla (\rho_v \nu_a) - C_{pi}\rho_i \nabla \left[ \nu_i \left( T - T_v \right) \right] - C_{pv} \nabla \left[ \rho_v \nu_v \left( T - T_v \right) \right] \]

\[ - \nabla \left[ \rho_v \nu_v \left( T - T_v \right) \right] - \nabla \left[ \rho_{da} \nu_a \left( T - T_v \right) \right] = \nabla \left( K_T \nabla u_t \right) + \nabla \left( K_{TT} \nabla T \right) + \nabla \left( K_{Ta} \nabla u_a \right) \]

+ J_r

(3.98)

where;

\[ K_T = L \rho_i \frac{D_{aim} \nu_n}{\rho_i} \left( \rho_0 \frac{\partial H}{\partial \xi} \right) + \left( T - T_v \right) \rho_i \left( C_{pi} k_i \rho_i / \gamma_i + C_{pv} \frac{D_{aim} \nu_n}{\rho_i} \left( \rho_0 \frac{\partial H}{\partial \xi} \right) \right) \]

(3.99)

\[ K_{TT} = \lambda_T + L \rho_i \frac{D_{aim} \nu_n (\nabla T)_t}{\rho_i \nabla T} \left( h \frac{\partial \rho_0}{\partial T} + \rho_0 \frac{\partial H}{\partial T} \right) \]

+ \left( T - T_v \right) \rho_i C_{pi} \frac{D_{aim} \nu_n (\nabla T)_t}{\rho_i \nabla T} \left( h \frac{\partial \rho_0}{\partial T} + \rho_0 \frac{\partial H}{\partial T} \right) \]

(3.100)

\[ K_{Ta} = -L \rho_i \frac{D_{aim} \nu_n}{\rho_i} \left( \rho_0 \frac{\partial H}{\partial \xi} \right) + L \rho \cdot k_a \]

\[ \left( T - T_v \right) \left( - \rho_i C_{pv} \frac{D_{aim} \nu_n}{\rho_i} \left( \rho_0 \frac{\partial H}{\partial \xi} \right) + \rho_v C_{pv} k_a + \rho_{da} C_{pda} k_a \right) \]

(3.101)
\[ J_T = (T - T_r)C_p \rho_i \nabla (k_i \nabla z) \]  

(3.102)

Combining Equations (3.93) and (3.98) yields the governing differential equation for conservation of energy, in terms of primary variables as:

\[ C_n \frac{\partial u_i}{\partial t} + C_{TT} \frac{\partial T}{\partial t} + C_{nu} \frac{\partial u_n}{\partial t} + C_{nu} \frac{\partial u_n}{\partial t} = \nabla [K_n \nabla u_i] + \nabla [K_T \nabla T] + \nabla [K_n \nabla u_n] + J_T \]

(3.103)

3.5 Deformation behaviour

This section presents a theoretical approach to predict the deformation and swelling characteristics of expansive soils. The formulation is based on the elasto-plastic constitutive model developed by Alonso et al. (1990). The formulation has been presented earlier by Ramesh (1996), Thomas and He (1998), Cleall (1998) and Mitchell (2002). For the sake of brevity, a brief description of the model has been presented here.

Deformation is assumed to be a result of stress, suction and temperature change. Deformation due to changes in osmotic potential is ignored in this formulation. Adopting the approach set out in Alonso et al. (1990), an elasto-plastic work hardening constitutive model is produced by considering net mean stress and suction as the relevant stress variables. The net mean stress is defined as:

\[ \sigma^* = \sigma - u_a \]  

(3.104)

where \( \sigma \) represents the total stress. In this work a positive sign is taken as tension for stress but the pore pressures, \( u_i \), and \( u_a \) are defined as positive in compression.

For an element of soil with unit length and a cross sectional area of \( dxdz \) under a system of two-dimensional stresses and body forces (Figure 3.1), the stress equilibrium equation in an incremental form can be represented as:

\[ P d\sigma^* + P mdu_a + dB = 0 \]  

(3.105)

where \( b \) is the vector of body forces and \( P \) is the strain matrix given as:
\[
P = \begin{bmatrix}
\frac{\partial}{\partial x} & 0 & \frac{\partial}{\partial x} & 0 \\
0 & \frac{\partial}{\partial z} & \frac{\partial}{\partial z} & 0
\end{bmatrix}
\]

(3.106)

For a two dimensional plane stress or plane strain analysis, the vector \( \mathbf{m} \) is defined as:

\[
\mathbf{m}^T = (1, 1, 0, 0)
\]

(3.107)

For axisymmetric analysis, and three dimensional analysis:

\[
\mathbf{m}^T = (1, 1, 0, 1)
\]

(3.108)

### 3.5.1 Stress-Strain relationship

The stress strain relationship can be described using the generalised Hooke’s law:

\[
d\sigma = \mathbf{D} d\varepsilon
\]

(3.109)

where \( d\varepsilon \) represents the incremental strain and \( \mathbf{D} \) represents the elasticity matrix.

For a soil exhibiting elasto-plastic behaviour, an increment of stress would be accompanied by a change of strain \( d\varepsilon \), which is assumed to be divisible into elastic and plastic components (Owen and Hinton, 1980). Hence, the incremental strain can be expressed as:

\[
d\varepsilon = d\varepsilon^e + d\varepsilon^p
\]

(3.110)

where \( d\varepsilon^e \) is the incremental elastic component of strain, and \( d\varepsilon^p \) is the incremental plastic component of strain.

The approach taken by Wang (1953) was extended by Thomas and He (1995), so that the incremental elastic strain may be written as:

\[
d\varepsilon^e = d\varepsilon^e_p + d\varepsilon^e_s + d\varepsilon^e_t
\]

(3.111)

where \( \varepsilon \) is the strain vector, and the subscripts \( p, s, \) and \( T \) represent the components due to change in stress, suction, and temperature respectively.
Substituting Equations (3.110) and (3.111) into (3.109), the stress-strain relationship can be expressed as:

\[ d\sigma^* = D(d\varepsilon - d\varepsilon^e - d\varepsilon^p) \]  

(3.112)

The following sections deal with the determination of both elastic and plastic strains.

3.5.2 Elasto-plastic constitutive relationships

Observing Equation (3.112), deformation relationships need to be established to determine the elastic and plastic strain components. According to Britto and Gunn (1987) the relationships required have been identified as: a stress/elastic strain relationship, a yield criterion, a flow rule to define the magnitude of plastic strains when yield point is reached, and a hardening rule.

The following sections identify the approach taken to establish the deformation relationships for this works.

3.5.2.1 Material behaviour under elastic condition

Figure 3.2 shows the compression curves of a soil sample subjected to isotropic compression tests. The idealised virgin compression curves are shown to have a slope gradient of \(-\lambda\) and the swelling and recompression curves have a slope of \(-\kappa\). During the swelling and recompression phase, it is assumed that soil deforms elastically (Alonso et al., 1990).

According to Schofield and Wroth (1968) the change in specific volume for an elastic region due to incremental stress change at constant suction can be represented as:

\[ dv = -\kappa \frac{dp}{p} \]  

(3.113)

Thus, the elastic volumetric strain component due to stress changes can be obtained as:

\[ d\varepsilon^e_p = \frac{dv}{v} = -\frac{\kappa}{v} \frac{dp}{p} \]  

(3.114)
Rewriting the equation to define the change in specific volume due to suction changes and adding the term $p_{\text{atm}}$ to avoid infinite values of strain as suction approaches zero, gives:

$$d\varepsilon_p^e = - \frac{K_r}{\nu} \frac{ds}{(s + p_{\text{atm}})} = A_s ds$$  \hspace{1cm} (3.115)$$

The dependence of suction on temperature has been discussed in Section 3.2. It is clear that the volumetric strain due to temperature change should include contributions from suction changes and thermal expansion (Wang, 1953):

$$d\varepsilon_T^e = \alpha_T \frac{dT}{v_0} \left( A_s + A_s \frac{\partial s}{\partial T} \right) dT$$  \hspace{1cm} (3.116)$$

where $\alpha_T$ is the coefficient of thermal expansion, and $v_0$ is the initial specific volume.

The incremental deviatoric strain caused by changes in deviatoric stress can be expressed as, (Wood, 1990):

$$d\varepsilon_q^e = \frac{1}{3G} dq$$  \hspace{1cm} (3.117)$$

where $q$ is the deviatoric stress and $G$ is the shear modulus.

**3.5.2.2 Yield function**

The yield criterion determines the point in stress space at which yielding occurs. Two yield functions, the loading-collapse (LC) curve and the suction-increase (SI) curve were proposed by Alonso et al. (1990) to represent two yield functions. The LC curve indicates that yielding occurs when preconsolidation stress reaches a critical point, $p_0$. The SI curve indicates another scenario where yield occurs when suction reaches a critical value, $s_0$. Both yield functions can be mathematically represented as:

$$F_1(p, q, s, p_0^*) = q^2 - M^2 (p + p_s)(p_0 - p) = 0$$  \hspace{1cm} (3.118)$$

$$F_2(s, s_0) = s - s_0 = 0$$  \hspace{1cm} (3.119)$$
where $q$ represents the deviatoric stress, $M$ represents the slope of the critical state line, $p_0$ represents the preconsolidation stress, $p_s$ represents the suction effect on the cohesion of the soil, and $s_0$ is the previously attained maximum value of suction.

Alonso et al. (1990) proposed the following equation, which defines the set of yield $p_0$ values for each associated suction:

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

(3.120)

where $p_0^*$ is the preconsolidation stress of saturated soil, $p_c$ is the reference stress, $\lambda(s)$ is the stiffness parameter for changes in net mean stress for virgin states of the soil and $\lambda(0)$ is the stiffness parameter for changes in net mean stress for virgin states of saturated soil.

An asymptotic expression is used to define the virgin soil stiffness parameter, $\lambda(s)$ (Alonso et al., 1990):

$$\lambda(s) = \lambda(0)\left[1 - r\right]$$

(3.121)

where $\beta$ is a parameter controlling the rate of increase of soil stiffness with suction, and the parameter $r$ controls the maximum stiffness of the soil. Figure 3.3 illustrates a graphical representation of these relationship in terms of the $(p,s)$ and $(p,v)$ space. The LC and SI yield curves in $(p,q)$, and $(p,s)$ space are shown graphically in Figures 3.4a and 3.4b.

3.5.2.3 Flow rule

Flow rule is needed to define the amount of plastic strains a material produces when it starts to yield. Two types of flow rules have been proposed by Alonso et al., (1990): an associated plastic flow rule for the SI surfaces and a non-associated flow rule for the LC yield surface.

The plastic potential for LC yield surface Q1, as defined by non-associated flow rule is:
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\[ Q_1 = \alpha_q q^2 - M^2(p + p_s)(p_0 - p) \]  

(3.122)

The plastic potential for SI yield surface Q2, as defined by associated flow rule is,

\[ Q_2 = s - s_0 \]  

(3.123)

In this work, the plastic strain increment is assumed to be proportional to the stress gradient of the plastic potential. The plastic strain increment associated with yield surface F1 is represented by \( (d\varepsilon_{pl}^p, d\varepsilon_q^p) \), where;

\[ d\varepsilon_{pl}^p = \chi_1 \frac{dQ_1}{dp} = \chi_1 M^2(2p + p_s - p_0) \]  

(3.124)

\[ d\varepsilon_q^p = \chi_1 \frac{dQ_1}{dq} = \chi_1 2\alpha_q q \]  

(3.125)

The plastic strain increment associated with yield surface F2 is \( (d\varepsilon_{pl}^p, 0) \),

\[ d\varepsilon_{pl}^p = \chi_2 \frac{dQ_2}{ds} = \chi_2 \]  

(3.126)

where \( \chi_1 \) and \( \chi_2 \) are plastic multipliers, determined through plastic consistency conditions (Alonso et al., 1990).

The constant \( \alpha_q \) in Equation (3.122) is defined as (Alonso et al., 1990):

\[ \alpha_q = \frac{M(M - 9)(M - 3)}{6(6 - M)} \frac{1}{\left(1 - \frac{\kappa}{\kappa(0)}\right)} \]  

(3.127)

3.5.2.4 Hardening laws

Josa et al. (1987) found a coupling relationship between the hardening of the two yield surfaces. The yield surfaces are influenced by the hardening parameters, \( p_0 \) and \( s_q \), which are dependent on the plastic volumetric strain increment, \( d\varepsilon^P \). The two hardening laws for the yield surfaces \( F_1 \) and \( F_2 \), are respectively, (Alonso et al., 1990);
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#### 3.5.3 Governing equation for deformation

As shown previously in Section 3.3.1 the elastic stress-strain relationship can be described by the use of elastic incremental constitutive matrix $D$. However, this form of stiffness matrix is not suitable to predict the change in stress when yielding occurs and requires further modification to take into the plastic strain. Adopting the approach proposed by Owen and Hinton (1980):

$$d\sigma = Dep\,d\varepsilon \quad (3.130)$$

The elasto-plastic stress-strain matrix, $Dep$ can be defined as (Mitchell, 2002):

$$Dep = D - \frac{D}{\sigma} \frac{\partial F_1}{\partial \sigma} D + \left( \frac{\partial Q_i}{\partial \sigma} \right)^T D \frac{\partial F_i}{\partial \sigma} \quad (3.131)$$

where $A$ is the plastic modulus defined as:

$$A = M^2(p + p_s) \frac{\lambda(0) - \kappa}{\lambda(s) - \kappa} p_0 \frac{\nu}{\lambda(0) - \kappa} \left( M^2(2p + p_s - p_0) \right) \quad (3.132)$$

The stress-strain relationship given in equation (3.112) may now be rewritten by splitting the total plastic strain increment into the sum of plastic strain increments due to stress and suction changes:

$$d\sigma^* = Dep(d\varepsilon - d\varepsilon^e - d\varepsilon^s - d\varepsilon^p) \quad (3.133)$$

Substitution of equations (3.115) and (3.116) into equation (3.133) gives:

$$d\sigma^* = Dep(d\varepsilon - A_x ds - (A_x + A_s \frac{dS}{dT})dT - d\varepsilon^p) \quad (3.134)$$

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Equation (3.105) can be rewritten with substitution from Equation (3.134), giving:

\[
P \left( \text{Dep} \left( P^T du + A_s du_s - \left( A_T + A_s \frac{dS_s}{dt} \right) dT - A_s du_a - d\varepsilon_s^p \right) \right) + Pm du_a + db = 0
\]

(3.135)

The governing differential equation for this approach can then be written as:

\[
C_u du_i + C_uT dT + C_u u du_a + C_u a du - \text{Dep} d\varepsilon_s^p + db = 0
\]

(3.136)

where;

\[
C_u = \text{Dep} A_s
\]

(3.137)

\[
C_uT = \text{Dep} \left( -A_T - A_s \frac{dS_s}{dT} \right)
\]

(3.138)

\[
C_uu = -\text{Dep} A_s + mP
\]

(3.139)

\[
C_u = \text{Dep} P^T
\]

(3.140)

3.6 Conclusions

The govern equations to describe the moisture flow, heat and air transfer in a deformable unsaturated soil have been developed and presented in the above sections. These equations have been formulated in terms of pore water pressure \((u_i)\), pore air pressure \((u_a)\), temperature \((T)\), and deformation \((u)\).

3.7 References


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Preece, R.J., (1975) “The measurement and calculation of physical properties of cable bedding sands. Part 2; specific thermal capacity, thermal conductivity and temperature ratio across ‘air’ filled pores”, C.E.G.B. Laboratory Note No., RD/L/N 231/74.

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Figure 3.1 A general two dimensional stress system
Figure 3.2  
(a) Typical isotropic compression and recompression curves 
(b) Idealised curves
Figure 3.3  

a) Compression curves for saturated and unsaturated soil  
b) Stress path and yield surface in \((p,s)\) space
Figure 3.4  

a) Yield surfaces in $(p,q)$ space  
b) Yield surfaces in $(p,s)$ space
Figure 3.5 Three dimensional view of yield surfaces in the \((p,q,s)\) space
Chapter 4

Finite element formulation

4.1 Introduction

In the previous chapter, governing differential equations describing moisture, air and heat flow in a deformable unsaturated soil were presented. In order to solve these equations, a numerical approach is employed. The finite element method is applied to spatially discretise the equations, and a finite difference time-stepping algorithm is applied to achieve temporal discretisation. The formulation of this solution is shown in this chapter.

4.2 Spatial discretisation

In this study the Galerkin weighted residual approach is employed. Further details regarding this approach have been presented in Zienkiewicz and Taylor (1991). The approach has been employed and found to be effective in many numerical modelling exercises (Thomas and He, 1995; Thomas et al., 1998; Cleall, 1998; Mitchell, 2002). To facilitate the readers' understanding on the numerical approach, a concise form of the spatial discretisation of the governing equations is presented here.

4.2.1 Spatial discretisation of the governing equations for flow variables

The process of spatial discretisation for moisture flow governing equation is shown in this section. As the discretisation process is similar for other types of flow, they will not be presented here.
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Finite element formulation

The shape function for an eight-noded element is used to estimate the primary unknowns and the derivatives. This gives the following:

\[ u_{\text{var}} = \hat{u}_{\text{var}} = \sum_{s=1}^{8} N_s \hat{u}_{\text{var}_s} \]  
\[ \nabla \hat{u}_{\text{var}} = \sum_{s=1}^{8} (\nabla N_s) \hat{u}_{\text{var}_s} \]

where \( \hat{u}_{\text{var}} \) represents any of the primary variables, \( (u, T, u_a, u) \), \( N_s \) is the shape function, the subscript \( s \) represents nodal points and the symbol, \(^\wedge\), signifies an approximate form.

Substituting the primary unknowns for the shape function approximations of equations (4.1) and (4.2), the governing differential equation for moisture flow, may be rewritten as;

\[
\left[-C_{ii} \frac{\partial \hat{u}_i}{\partial \alpha} - C_{ir} \frac{\partial \hat{T}}{\partial \alpha} - C_{ia} \frac{\partial \hat{u}_a}{\partial \alpha} - C_{iu} \frac{\partial \hat{u}}{\partial \alpha} + \right] = R_{\Omega} 
\]

\[
\nabla \left[ K_{ii} \nabla \hat{u}_i \right] + \nabla \left[ K_{ir} \nabla \hat{T} \right] + \nabla \left[ K_{ia} \nabla \hat{u}_a \right] + J
\]

where \( R_{\Omega} \) is the residual error introduced by substitution of the approximate values of the variables.

Employing the Galerkin weighted residual approach, the error is minimised over the elemental volume. For example;

\[
\int_{\Omega_e} N_s \left[-C_{ii} \frac{\partial \hat{u}_i}{\partial \alpha} - C_{ir} \frac{\partial \hat{T}}{\partial \alpha} - C_{ia} \frac{\partial \hat{u}_a}{\partial \alpha} - C_{iu} \frac{\partial \hat{u}}{\partial \alpha} + \right] \nabla \left[ K_{ii} \nabla \hat{u}_i \right] + \nabla \left[ K_{ir} \nabla \hat{T} \right] + \nabla \left[ K_{ia} \nabla \hat{u}_a \right] + J \, d\Omega_e = 0
\]

Employing integration by parts yields the weak form of Equation (4.4). For example, the fifth term can be expressed as;

\[
\int_{\Omega'} [N_s \nabla (K_s \nabla \hat{u}_i)] d\Omega_e = \int_{\Omega'} [N_s \nabla \hat{u}_i] d\Omega_e - \int_{\Omega'} [K_s \nabla \hat{u}_i \nabla N_s] d\Omega_e
\]

Similarly, the eighth term \( J \) can be expressed, with substitution from Chapter 3, as;

4-2
\[ \int_{\Omega^e} \left[ N, [J] \right] \Omega^e = \int_{\Omega^e} N, \rho_i \nabla [k_i \nabla z] \Omega^e \]
\[ = \int_{\Omega^e} \nabla (N, \rho_i k_i \nabla z) \Omega^e - \int_{\Omega^e} k_i \rho_i \nabla z \nabla N, d\Omega^e \]  

(4.6)

Integrating the remaining terms and rearranging, Equation (4.4) can be expressed as;

\[ \int_{\Omega^e} \left[ \nabla (N, K_{ii} \nabla w_i) - K_{ii} \nabla w_i \nabla N_r + \nabla (N, K_{i\gamma} \nabla \hat{T}) - K_{i\gamma} \nabla \hat{T} \nabla N_r, \\
+ \nabla (N, K_{\alpha\alpha} \nabla w_\alpha) - K_{\alpha\alpha} \nabla w_\alpha \nabla N_r + \nabla (N, \rho_i K_i \nabla z) - k_i \rho_i \nabla z \nabla N_r, \right] d\Omega^e = 0 \]

(4.7)

The Gauss-Green Divergence theorem is applied to reduce the second order terms to first order terms. Although this approach introduces surface integrals, adjacent elements will cancel these integrals and leave only a contribution on the limit of the domain. Equation (4.7) can then be expressed as;

\[ \int_{\Omega^e} \left[ - K_{ii} \nabla w_i \nabla N_r - K_{i\gamma} \nabla \hat{T} \nabla N_r, \\
- K_{\alpha\alpha} \nabla w_\alpha \nabla N_r - k_i \rho_i \nabla z \nabla N_r, \\
- N_r \left[ C_{ii} \frac{\partial w_i}{\partial t} + C_{i\gamma} \frac{\partial \hat{T}}{\partial t} \\
+ C_{\alpha\alpha} \frac{\partial w_\alpha}{\partial t} + C_{ii} \frac{\partial w_i}{\partial t} \right] \right] d\Omega^e + \int_{\Gamma^e} \left[ N_r \left[ K_{ii} \nabla w_i + K_{i\gamma} \nabla \hat{T} + k_i \rho_i \nabla z \right] \right] n d\Gamma^e = 0 \]

(4.8)

where \( \Gamma^e \) is the element boundary surface and \( n \) is the direction cosine normal to the surface. As the surface integral in Equation (4.8) is equal to the sum of the liquid and the vapour flux normal to the boundary surface, this may be expressed as;
\[ \int_{\Gamma^e} \left[ N^T \left( K_{\tau} \nabla \hat{u}_T + K_{\gamma} \nabla \hat{T} + K_{\nu \alpha} \nabla \hat{u}_\alpha + k_1 \rho_1 \nabla z \right) \right] d\Gamma^e \]

\[ = \int_{\Gamma^e} \left[ N^T \left( \rho_1 k_1 \left( \frac{1}{\gamma_1} \nabla \hat{u}_T + \nabla z \right) + \rho_1 \left( K_{\nu} \nabla \hat{u}_T + K_{\gamma} \nabla \hat{T} + K_{\nu \alpha} \nabla \hat{u}_\alpha \right) + \rho_1 \left( k_{\nu} \nabla \hat{u}_\alpha \right) \right) \right] d\Gamma^e \]

\[ = \int_{\Gamma^e} \left[ N^T \left( \rho_1 \hat{v}_l + \rho_1 \hat{v}_{vd} + \rho_1 \hat{v}_{va} \right) \right] d\Gamma^e \]

(4.9)

where \( \hat{v}_l \) is the approximate liquid velocity normal to the boundary surface, \( \hat{v}_{vd} \) is the approximate diffusive vapour velocity normal to the boundary surface, \( \hat{v}_{va} \) is the approximate pressure vapour velocity normal to the boundary surface, and;

\[ K_{vd} = \frac{D_{ama} v_r n}{\rho_1} \left( \rho_0 \frac{\partial h}{\partial s} \right) \]

(4.10)

\[ K_{\nu T} = -\frac{D_{ama} v_r n}{\rho_1} \left( \frac{\nabla T}{\nabla \nu} \right) \left[ \frac{\partial \rho_0}{\partial T} + \rho_0 \frac{\partial h}{\partial T} \right] \]

(4.11)

\[ K_{\nu \alpha} = -\frac{D_{ama} v_r n}{\rho_1} \left( \rho_0 \frac{\partial h}{\partial s} \right) \]

(4.12)

Introducing the expressions for the derivatives of the primary variables yields;

\[ \int_{\Omega^e} \left[ K_{\nu} \nabla N^T \nabla N \right] d\Omega^e u_{ls} + \int_{\Omega^e} \left[ K_{\gamma} \nabla N^T \nabla N \right] d\Omega^e T_s + \int_{\Omega^e} \left[ K_{\nu \alpha} \nabla N^T \nabla N \right] d\Omega^e u_{as} \]

\[ + \int_{\Omega^e} \left[ C_{\nu} N^T N \right] d\Omega^e \frac{\partial u_{ls}}{\partial t} + \int_{\Omega^e} \left[ C_{\gamma} N^T N \right] d\Omega^e \frac{\partial T_s}{\partial t} + \int_{\Omega^e} \left[ C_{\nu \alpha} N^T N \right] d\Omega^e \frac{\partial u_{as}}{\partial t} \]

\[ + \int_{\Omega^e} \left[ C_{\nu \alpha} N^T N \right] d\Omega^e \frac{\partial u_{as}}{\partial t} + \int_{\Omega^e} \left[ k_{\nu} \rho_1 \nabla N^T \nabla z \right] d\Omega^e \]

\[ - \int_{\Gamma^e} \left[ N^T \left( \rho_1 \hat{v}_l + \rho_1 \hat{v}_{vd} + \rho_1 \hat{v}_{va} \right) \right] d\Gamma^e = 0 \]

(4.13)

where \( N \) is the shape function matrix, \( u_{ls} \) is the pore water pressure vector, \( T_s \) is the temperature vector \( u_{as} \) is the pore air pressure vector, and \( u \) is displacement vector.

Rewriting this in the form of a concise matrix notation yields;
Chapter 4 Finite element formulation

\[
C_u \frac{\partial u_{i2}}{\partial t} + C_{\tau u} \frac{\partial T_{j}}{\partial t} + C_{\tau a} \frac{\partial u_{a2}}{\partial t} + C_{\tau u} \frac{\partial u_{j}}{\partial t} + K_{\tau u} u_{i2} + K_{\tau} T_{j} + K_{\tau a} u_{a2} = f_{i}
\] (4.14)

where;

\[
C_u = \sum_{e=1}^{m} \int [C_{u} N^T N] d\Omega^e
\] (4.15)

\[
C_{\tau u} = \sum_{e=1}^{m} \int [C_{\tau u} N^T N] d\Omega^e
\] (4.16)

\[
C_{\tau a} = \sum_{e=1}^{m} \int [C_{\tau a} N^T N] d\Omega^e
\] (4.17)

\[
C_{\tau u} = \sum_{e=1}^{m} \int [C_{\tau u} N^T N] d\Omega^e
\] (4.18)

\[
K_{\tau u} = \sum_{e=1}^{m} \int [K_{\tau u} \nabla N^T \nabla N] d\Omega^e
\] (4.19)

\[
K_{\tau} = \sum_{e=1}^{m} \int [K_{\tau} \nabla N^T \nabla N] d\Omega^e
\] (4.20)

\[
K_{\tau a} = \sum_{e=1}^{m} \int [K_{\tau a} \nabla N^T \nabla N] d\Omega^e
\] (4.21)

\[
f_{i} = \sum_{e=1}^{m} \int \left[ k_{i} \rho_{i} \nabla N^T \nabla z \right] d\Omega^e - \sum_{e=1}^{m} \int N^T m \left[ \rho_{i} \dot{\phi}_{ln} + \rho_{i} \dot{\phi}_{va} + \rho_{e} \dot{\phi}_{va} \right] d\Omega^e
\] (4.22)

The above process may be repeated for the other flow variables \((T, u_{a})\) producing for:

Heat transfer

\[
C_{\tau T} \frac{\partial u_{i2}}{\partial t} + C_{\tau T} \frac{\partial T_{j}}{\partial t} + C_{\tau a} \frac{\partial u_{a2}}{\partial t} + C_{\tau u} \frac{\partial u_{j}}{\partial t} + K_{\tau T} u_{i2} + K_{\tau} T_{j} + K_{\tau a} u_{a2} = f_{T}
\] (4.23)

where;
\begin{align*}
C_{\Omega} & = \sum_{e=1}^{m} \int_{\Omega_e} \left[ C_{\Omega} N^T N \right] d\Omega^e \\
C_{TT} & = \sum_{e=1}^{m} \int_{\Omega_e} \left[ C_{TT} N^T N \right] d\Omega^e \\
C_{Ta} & = \sum_{e=1}^{m} \int_{\Omega_e} \left[ C_{Ta} N^T N \right] d\Omega^e \\
C_{Ta} & = \sum_{e=1}^{m} \int_{\Omega_e} \left[ \frac{\partial C_{Ta}}{\partial u} N^T N \right] d\Omega^e \\
K_{n} & = \sum_{e=1}^{m} \int_{\Omega_e} \left[ K_{n} \nabla N^T \nabla N \right] d\Omega^e \\
K_{TT} & = \sum_{e=1}^{m} \int_{\Omega_e} \left[ K_{TT} \nabla N^T \nabla N \right] d\Omega^e \\
K_{Ta} & = \sum_{e=1}^{m} \int_{\Omega_e} \left[ K_{Ta} \nabla N^T \nabla \nabla + \nabla^T V_{n} \nabla N \right] d\Omega^e \\
f_{e} & = \sum_{e=1}^{m} \int_{\Omega_e} \left[ f_{e} \nabla N^T \nabla \right] d\Omega^e - \sum_{e=1}^{m} \int_{\Omega_e} \left[ F_{h} \right] d\Omega^e \\
\end{align*}

In the above, $F_{h}$ is the approximate heat flux normal to the boundary surface.

**Air transfer**

\begin{align*}
C_{st} \frac{\partial u_{s}}{\partial t} + C_{st} \frac{\partial T_{s}}{\partial t} + C_{as} \frac{\partial u_{a}}{\partial t} + C_{su} \frac{\partial u_{s}}{\partial t} + K_{as} u_{s} + K_{u} u_{a} + K_{u_{a}} u_{a} &= f_{a} \\
\end{align*}

where;

\begin{align*}
C_{st} & = \sum_{e=1}^{m} \int_{\Omega_e} \left[ C_{st} N^T N \right] d\Omega^e \\
C_{as} & = \sum_{e=1}^{m} \int_{\Omega_e} \left[ C_{as} N^T N \right] d\Omega^e \\
\end{align*}
\[ C_{ss} = \sum_{e=1}^{m} \int \left[ C_{ss} N^T N \right] d\Omega^e \]  
\[ C_{su} = \sum_{e=1}^{m} \int \left[ C_{su} N^T N \right] d\Omega^e \]  
\[ K_{si} = \sum_{e=1}^{m} \int \left[ K_{si} \nabla N^T \nabla N \right] d\Omega^e \]  
\[ K_{su} = \sum_{e=1}^{m} \int \left[ K_{su} \nabla N^T \nabla N \right] d\Omega^e \]  
\[ f_s = \sum_{e=1}^{m} \int \left[ k_{i} \rho_{ds} \nabla N^T \nabla z \right] d\Omega^e - \sum_{e=1}^{m} \int N^T \rho_{ds} (\hat{v}_{fn} + \hat{v}_{an}) d\Omega^e \]  

In the above, \( \hat{v}_{fn} \) and \( \hat{v}_{an} \) are the approximate velocities of free and dissolved air flux normal to the boundary surface.

### 4.2.2 Spatial discretisation of governing equations for displacement variables

Essentially, the spatial discretisation of the governing equations for deformation is similar to that for the flow variables. The development of the governing equation for deformation in an elasto-plastic swelling soil is presented here.

The governing equation for this approach was previously described in Chapter 3 as;

\[ C_{u} du_i + C_{u} dT + C_{uu} du_a + C_{uu} d\mathbf{u} - P Dep\varepsilon_i^p + db = 0 \]  

Using the shape function approach and substituting Equations (4.1) and (4.2) into Equation (4.40) gives;

\[ C_{a} \ddot{u}_i + C_{a} \dot{T} + C_{aa} \ddot{u}_a + C_{aa} \dot{\mathbf{u}} - P Dep\varepsilon_i^p + db = R_{\Omega} \]  

The Galerkin weighted residual approach is applied to minimise the error over the elemental volume as demonstrated;
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\[
\int_{\Omega^e} \left[ N_r \left( C_{\varepsilon} \dot{\varepsilon} + C_{\varepsilon} T + C_{\varepsilon} d\varepsilon + C_{\varepsilon} \dot{\varepsilon} - P \text{Dep} \varepsilon, + d\mathbf{b} \right) \right] d\Omega^e = 0
\]  
(4.42)

Integration by parts may be used to yield the weak form of equation (4.42). The first term of the equation may be written as;

\[
\int_{\Omega^e} N_r C_{\varepsilon} \dot{\varepsilon} d\Omega^e = \int_{\Omega^e} N_r \left[ P \text{Dep} \varepsilon, \right] d\varepsilon + d\mathbf{b} \right] d\Omega^e
\]

\(= - \int_{\Omega^e} \left[ P N_r \left[ \text{Dep} \varepsilon, \right] d\varepsilon + \int_{\Omega^e} \left[ P \left[ N_r \right] \text{Dep} \varepsilon, \right] d\varepsilon \)

where, P, N, and can be mathematically written as;

\[
B = \begin{bmatrix}
\frac{\partial N_r}{\partial x} & 0 \\
0 & \frac{\partial N_r}{\partial z} \\
\frac{\partial N_r}{\partial z} & \frac{\partial N_r}{\partial x} \\
0 & 0
\end{bmatrix}
\]  
(4.44)

Considering the second term of Equation (4.42), integration by parts yields;

\[
\int_{\Omega^e} N_r C_{\varepsilon} T d\Omega^e = \int_{\Omega^e} N_r \left[ P \text{Dep} \left( - A_r - A_s \frac{dS_r}{dt} \right) \right] d\varepsilon + d\mathbf{b} \right] d\Omega^e
\]

\(- \int_{\Omega^e} \left[ B \text{Dep} \left( - A_r - A_s \frac{dS_r}{dt} \right) d\varepsilon + \int_{\Omega^e} \left[ P \left[ N_r \right] \text{Dep} \left( - A_r - A_s \frac{dS_r}{dt} \right) \right] d\varepsilon \)

\(= \int_{\Omega^e} N_r C_{\varepsilon} \dot{\varepsilon} d\Omega^e = \int_{\Omega^e} N_r \left[ P \text{Dep} \varepsilon, \right] d\varepsilon + d\mathbf{b} \right] d\Omega^e
\]

Considering the third term of Equation (4.42), integration by parts yields;

\[
\int_{\Omega^e} N_r C_{\varepsilon} \dot{\varepsilon} d\Omega^e = \int_{\Omega^e} N_r \left[ - P \text{Dep} \varepsilon, - m P \right] d\varepsilon + d\mathbf{b} \right] d\Omega^e
\]

\(- \int_{\Omega^e} \left[ B \left[ - \text{Dep} \varepsilon, - m \right] d\varepsilon + \int_{\Omega^e} \left[ P \left[ N_r \left[ - \text{Dep} \varepsilon, - m \right] d\varepsilon \right] d\varepsilon \)

Considering the fourth term of Equation (4.42), integration by parts yields;

\[
\int_{\Omega^e} N_r C_{\varepsilon} \dot{\varepsilon} d\Omega^e = - \int_{\Omega^e} \left[ B \text{Dep} \dot{\varepsilon} d\varepsilon + \int_{\Omega^e} \left[ P \left[ N_r \right] \text{Dep} \dot{\varepsilon} \right] d\varepsilon \)

\]
Considering the fifth term of Equation (4.42), integration by parts yields:

\[ \int_{\Omega^e} N_r \mathbf{P} \mathbf{D} \varepsilon_r d\Omega^e = - \int_{\Gamma^e} \mathbf{B} \mathbf{D} \mathbf{P} \varepsilon_r \mathbf{n} d\Gamma^e + \int_{\Omega^e} \mathbf{P} \left[ \mathbf{N} \mathbf{D} \mathbf{p} \varepsilon_r \right] d\Omega^e \]  \hspace{1cm} \text{(4.48)}

Substituting Equations (4.43) to (4.48), into equation (4.42) yields:

\[ - \int_{\Omega^e} \mathbf{B} \left[ \mathbf{D} \mathbf{p} \varepsilon_r \mathbf{n} \right] d\Omega^e = \int_{\Gamma^e} \mathbf{P} \mathbf{N} \mathbf{D} \mathbf{p} \varepsilon_r \mathbf{n} d\Gamma^e + \int_{\Omega^e} \mathbf{P} \left[ \mathbf{N} \mathbf{D} \mathbf{p} \varepsilon_r \right] d\Omega^e + \int_{\Omega^e} \mathbf{N} d\mathbf{d} \Omega^e = 0 \]  \hspace{1cm} \text{(4.49)}

The Gauss-Green divergence theorem may then be applied to Equation (4.49), which yields the surface integrals.

\[ - \int_{\Gamma^e} \mathbf{B} \left[ \mathbf{D} \mathbf{p} \varepsilon_r \mathbf{n} \right] d\Gamma^e = \int_{\Gamma^e} \mathbf{P} \mathbf{N} \mathbf{D} \mathbf{p} \varepsilon_r \mathbf{n} d\Gamma^e + \int_{\Omega^e} \mathbf{P} \left[ \mathbf{N} \mathbf{D} \mathbf{p} \varepsilon_r \right] d\Omega^e + \int_{\Omega^e} \mathbf{N} d\mathbf{d} \Omega^e = 0 \]  \hspace{1cm} \text{(4.50)}
The surface integral in Equation (4.50) may be simplified as follows;

\[
\int_{\Gamma} [N, \text{Dep}_A] d\mathbf{u}, nd\Gamma^e + \int_{\Gamma} N, \text{Dep} \left( - A_r - A_s \frac{dS_r}{dt} \right) d\hat{T} nd\Gamma^e
\]

\[
+ \int_{\Gamma} \left[ N, \left( \text{Dep}_A - m \right) d\mathbf{u} \right] nd\Gamma^e + \int_{\Gamma} [N, \text{Dep}_P^T d\mathbf{u}] nd\Gamma^e - \int_{\Gamma} \left[ [N, \text{Dep}_P^T] \right] nd\Gamma^e
\]

\[
= \int_{\Gamma} \left[ \text{Dep}_A \left( d\mathbf{u}_r - d\mathbf{u}_a \right) - md\mathbf{u}_a + \text{Dep} \left( - A_r - A_s \frac{dS_r}{dt} \right) d\hat{T} \right] nd\Gamma^e = \int_{\Gamma} \left[ N, \hat{T}_r, d\Gamma^e \right]
\]

(4.51)

where, \( \hat{T}_r \) is the approximate traction.

Introducing the derivatives of shape functions as given in Equation (4.2), Equation (4.51) can be re-written as;

\[
- \int_{\Gamma} [B[\text{Dep}_A, N]] d\Omega^e d\mathbf{u}_{is} - \int_{\Gamma} B\text{Dep} \left( - A_r - A_s \frac{dS_r}{dt} \right) N d\Omega^e dT,
\]

\[
- \int_{\Gamma} [B[- \text{Dep}_A - m] N] d\Omega^e d\mathbf{u}_{as} - \int_{\Gamma} [B\text{Dep}\mathbf{B}^T] d\Omega^e d\mathbf{u}_a
\]

\[
+ \int_{\Gamma} [B\text{Dep}_P^T] d\Omega^e + \int_{\Gamma} [N^T d\mathbf{b}] d\Omega^e + \int_{\Gamma} \hat{T}_r d\Gamma^e = 0
\]

(4.52)

The incremental form of the Equation (4.52) can be used during transient analysis. This is achieved by multiplying the constants by the gradient of time. Thus, Equation (4.52) may be written in concise matrix notation as;

\[
C_{u_1} \frac{\partial \mathbf{u}_{is}}{\partial t} + C_{u_2} \frac{\partial \mathbf{T}}{\partial t} + C_{u_3} \frac{\partial \mathbf{u}_{as}}{\partial t} + C_{u_4} \frac{\partial \mathbf{u}_a}{\partial t} = f_u
\]

(4.53)

\[
C_{u_1} = \sum_{e=1}^m \int_{\Gamma_e} [B[\text{Dep}_A, N]] \nabla_t d\Omega^e
\]

(4.54)

\[
C_{u_2} = \sum_{e=1}^m \int_{\Gamma_e} B\text{Dep} \left[ - A_r - A_s \frac{dS_r}{dt} \right] N \nabla_t d\Omega^e
\]

(4.55)

\[
C_{u_3} = \sum_{e=1}^m \int_{\Gamma_e} [B[- \text{Dep}_A - m] N] \nabla_t d\Omega^e
\]

(4.56)
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\[ C_{uu} = \sum_{\alpha^e} \int_{\Omega^e} B B^T \nabla d\Omega^e \]  
\[ f_u = \sum_{\alpha^e} \left[ \int_{\Omega^e} B B^T \varepsilon \right] d\Omega^e + \int_{\Gamma^e} N^T d\Gamma^e + \int_{\Gamma^e} \mathbf{T}^e d\Gamma^e \]  

4.3 Temporal Discretisation Of The Coupled Flow And Deformation Formulation

The matrix form of the spatially discretised equations for the moisture, heat and air in a deformable soil is can be represented by:

\[
\begin{bmatrix}
K_{ll} & K_{lt} & K_{ls} & - & [u]_l \\
K_{tl} & K_{tt} & K_{ts} & - & T_s \\
K_{sl} & K_{st} & K_{ss} & - & [u]_s \\
- & - & - & - & [u]_a
\end{bmatrix}
\begin{bmatrix}
C_{ll} & C_{lt} & C_{ls} & C_{lu} & \dot{u}_l \\
C_{tl} & C_{tt} & C_{ts} & C_{tu} & \dot{T}_s \\
C_{sl} & C_{st} & C_{ss} & C_{su} & \dot{u}_a \\
C_{ul} & C_{ut} & C_{us} & C_{ua} & \dot{u}_a
\end{bmatrix}
\begin{bmatrix}
0 \\
0 \\
0 \\
0
\end{bmatrix} = 0
\]

where the terms involving deformation are specific for each of the three constitutive relationships proposed, based on the variables of temperature, suction and net stress.

The terms \( \dot{u}_a, \dot{T}_s, \dot{u}_s, \) and \( \dot{u}_s \) are the time differentials of the primary variables. As such, Equation (4.59) can be simplified to give:

\[ A\phi + B \frac{\partial \phi}{\partial t} + C = \{0\} \]

where \( \phi \) represents the variable vector.

The fully implicit mid-interval backward difference time-stepping algorithm is employed to achieve temporal discretisation. The general form of the algorithm is shown as;

\[ A^* \left[ \alpha \phi^{n+1} + (1 - \alpha) \phi^n \right] + B^* \left[ \frac{\phi^{n+1} - \phi^n}{\Delta t} \right] + C^* = \{0\} \]
Where $\sigma$ represents an integration constant ($\sigma = 1, 0.5, 0$ represent implicit, Crank-Nicholson and explicit time integration schemes respectively), the superscript $\phi_i$ represents the level at which the matrices $A$, $B$ and $C$ are evaluated, which is expressed as:

$$\phi_i = \sigma(n+1) + (1-\sigma)(n)$$  \hspace{1cm} (4.62)

where $\sigma$ is a constant which determines the level of evaluation. For the fully implicit mid-interval backward difference time-stepping algorithm, the constants $\omega$ and $\sigma$ take the values of 1 and 0.5 respectively.

Replacing these values into Equation (4.61) yields:

$$A^{n+1} \phi^{n+1} + B^{n+\frac{1}{2}} \frac{\phi^{n+1} - \phi^n}{\Delta t} + C^{n+\frac{1}{2}} = \{0\}$$  \hspace{1cm} (4.63)

Rearranging the above equation gives:

$$\phi^{n+1} = \left[ A^{n+\frac{1}{2}} + B^{n+\frac{1}{2}} \frac{\Delta t}{\Delta t} \right]^{-1} \left[ B^{n+\frac{1}{2}} \frac{\phi^n}{\Delta t} - C^{n+\frac{1}{2}} \right]$$  \hspace{1cm} (4.64)

The solution for the vector $\phi^{n+1}$ can be achieved via a predictor-corrector iterative approach. This is shown as follows:

1. A first estimate, named as the predictor, is produced by evaluating matrices $A$, $B$ and $C$ at time $n$.

2. Following that, both the predictor and previous time step values are used to evaluate $A$, $B$ and $C$ at time $n+\frac{1}{2}$. As a result, this estimate is known as the corrector.

3. If the analysis is for elasto-plastic case, a yield check is required. If the developed strain rate exceeds a specified tolerance, plastic strain will be produced and material hardening will be evaluated.

4. Either of the following conditions may then be used to check for convergence;
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\[ \phi_{ic}^{n+1} - \phi_{(i-1)c}^{n+1} \begin{bmatrix} TL_{abs} \end{bmatrix} \] (4.65)

\[ \phi_{ic}^{n+1} - \phi_{(i-1)c}^{n+1} \begin{bmatrix} TL_{rel} \end{bmatrix} \] (4.66)

where \( i \) is the iteration level, \( C \) represents the fact that it is a corrector value and \( TL_{abs} \) and \( TL_{rel} \) are the matrices of absolute and relative tolerances for each variable. The stress equilibrium will also be checked to ensure the residual force is within a tolerance value. Using the approach proposed by Owen and Hinton (1980), the residual force, \( \zeta \), can be calculated as;

\[ \int_B B^T \Delta \sigma d\Omega - \Delta F = \zeta \] (4.67)

where \( \Delta F \) is the increment of the applied force. If the variables do not converge, or the residual is too large, the algorithm returns to step 2. The corrector then becomes the new predictor.

5. When convergence is achieved, the algorithm moves onto the next time step and starts again from step 1.

The number of iterations required is dependent on the size of the time step in place. A variable time stepping scheme is applied to provide an efficient solution algorithm. Essentially, if the number of iterations exceeds a specified maximum the time step is decreased by a factor. Conversely, if the number of iterations is lower than a specified minimum then the time step size is increased by a factor.

4.4 Conclusions

The approach taken to arrive at a solution for the coupled flow and deformation formulation shown previously in Chapter 3 has been presented. Spatial discretisation of the four governing differential equations has been made possible using the finite element method. A backward difference mid-interval time stepping algorithm has been adopted to produce temporal discretisation. The model has been incorporated into COMPASS (COde for Modelling PArtially Saturated Soils), a computer code
developed at the Geoenvironmental Research Centre, Cardiff University (Thomas et al., 1998).

4.5 References


Chapter 5

Material Parameters

5.1 Introduction

The theoretical model described in Chapter 3 requires a set of thermo/hydro/mechanical parameters for each material found in the domain. This chapter sets out to describe the flow and deformation characteristics of the materials used in the analysis of the Buffer/Container Experiment and the In Room Emplacement.

Five different materials were used in AECL's Buffer/Container Experiment; a sand/bentonite buffer, the host granite rock, a bentonite based backfill, a sand annulus, and a layer of concrete. AECL's proposed layout for the In-Room Emplacement consists of ten different materials; a copper container, a bentonite based inner buffer, a bentonite based gap fill, a sand/bentonite outer buffer, a dense backfill which consists of bentonite, lake clay and aggregate, a sand/bentonite light backfill, an inner Excavation Damaged Zone (EDZ) rock layer, an outer EDZ rock layer, and granite host rock at near field and far field region.

Section 5.2 presents the thermo/hydro/mechanical parameters for the materials used in the Buffer/Container Experiment. Section 5.3 defines the parameters used to describe the materials used in the In Room Emplacement. Finally, the conclusions are presented in Section 5.4.
5.2 Buffer/Container Experiment

As described earlier, a set of thermo/hydro/mechanical parameters are required for the theoretical model. In this section, the flow and deformation relationships for the materials found in the Buffer/Container Experiment are described.

5.2.1 Sand/bentonite buffer

Compaction tests performed by Dixon and Gray (1985) led to the selection of a buffer material consisting of a 50:50 mixture (by dry weight) of silica sand and sodium bentonite mixed with water. The sand used was well graded fine to medium silica mixture, with 80% of the particles in the size range of 0.1 mm to 1.0 mm. The clay used was a natural sodium-based bentonite obtained from Southern Saskatchewan, Canada. The buffer was mixed to a gravimetric moisture content of 18% and a dry density of 1.76 Mg/m$^3$ with an initial porosity of 0.38. The water taken to mix the sand/bentonite was taken from the host granite rock. This would minimise any chemically induced swelling within the buffer and simplify the analysis of the results. The chemical composition of the ground water is described in Table 5.1.

5.2.1.1 Thermo/hydraulic parameters

Wan et al., (1995) carried out a series of experiments on unsaturated buffer material and concluded that the variation in total suction with water content was due to changes in the matric suction. The experimental data was fitted to a curve and is shown in Figure 5.1 (Graham et al., 1997). Following that, the initial porosity of the buffer material was used to describe a corresponding water retention curve. The curve may be represented using a set of equations. The water retention curve is graphically represented in Figure 5.2 and the equations are given as follow;

\[
S_t = 1 + 2.2625 \times 10^{-5} \left(1 - \exp\left(2.80 \times 10^{-6} \times s\right)\right) \quad s < 2.59 \text{ MPa} \quad (5.1)
\]

\[
S_t = -0.5329 \log_{10}(s) + 4.3856 \quad 2.59 \text{ MPa} < s < 17 \text{ MPa} \quad (5.2)
\]

\[
S_t = -0.3543 \log_{10}(s) + 3.0966 \quad 17 \text{ MPa} < s \quad (5.3)
\]
The unsaturated hydraulic conductivity curve was determined by applying the Green and Corey (1971) approach, using a measured saturated hydraulic conductivity of $1 \times 10^{-12}$ m/s (Graham et al., 1997). The relationship between degree of saturation and the hydraulic conductivity is shown in Figure 5.3 and applied in the finite element code COMPASS as a series of data points with linear interpolation being used between the discrete values.

The thermal conductivity relationship is based on experimental measurements presented by Wan et al., (1995). The experimental results plotted against gravimetric water content are shown in Figure 5.4. A series of straight lines may be fitted through the data as detailed below, (Graham et al., 1997).

\begin{align*}
\lambda &= 0.7 \text{ W/m/K} & S_t < 20\% \\
\lambda &= 1.667 S_t + 0.367 \text{ W/m/K} & 20\% < S_t < 80\% \\
\lambda &= 1.7 \text{ W/m/K} & 80\% < S_t
\end{align*}

(5.4) (5.5) (5.6)

The thermal conductivity relationship plotted against degree of saturation is shown in Figure 5.5. The specific heat capacity, $C_{p\text{soil}}$ and the thermal expansion coefficient for the buffer are given as 1400 J/kg.K and $2.3 \times 10^{-4}$/K respectively (Graham et al., 1997).

5.2.1.2 Mechanical parameters

A non-linear elastic model was used to model the mechanical behaviour of the inner buffer. The following principal data has been used for this model:

\begin{align*}
\kappa &= 0.0125 \\
\kappa_s &= 0.0111 \\
G &= 10 \text{ MPa}
\end{align*}

The values of $\kappa$ and $\kappa_s$ were taken from Mitchell (2002) who defined the mechanical parameters for the same sand/bentonite buffer. The shear modulus, $G$ for the sand/bentonite buffer was taken from Gens et al., (1998).
5.2.2 Granite rock material parameters

AECL’s underground research laboratory is situated in the Lac du Bonnet granite batholiths. A literature review carried out by Mitchell (2002) on the granite material parameters revealed there was little information available. Consequently, some assumptions have been made and are discussed as follow.

5.2.2.1 Thermo/hydraulic material parameters

Frieg and Vomvoris (1994) carried out laboratory experiments to determine the hydraulic properties of granite. The data was adopted by Gens et al., (1998) and an equation was fitted to it;

\[
S_l = \left[1 + \left(\frac{u_a - u_t}{P_0}\right)^{1/(1-\beta_t)}\right]^{-\beta_t} \quad \text{when} \quad u_a - u_t \geq 0 \tag{5.7}
\]

where \(S_l\) is the degree of saturation, \(u_a\) is the pore air pressure, \(u_t\) is the pore water pressure, \(\beta_t\) is a material coefficient, and \(P_0\) is the air entry value. The air entry value is defined as "the matric suction value that must be exceeded before air recedes into the soil pores" (Fredlund and Rahardjo, 1993). Gens et al., (1998) found that a material coefficient of 0.33 fitted the data for the granite investigated by Frieg and Vomvoris (1994). This value has also been adopted in this work. The air entry value chosen by Gens et al., (1998) was not adopted in this analysis as it was for a different type of granite rock.

A literature review carried out by Mitchell (2002) showed that Davies (1991) had proposed a relationship between intrinsic permeability and threshold pressure for a variety of geologic materials. This relationship is illustrated in Figure 5.6. According to Davies (1991), the threshold pressure can be defined as "the gas pressure required to overcome capillary resistance to initial gas penetration and the development of interconnected gas pathways that would allow outward gas flow". Comparing the definition of threshold pressure with that of the air entry value, it was therefore assumed that both terms could be considered equivalent. The saturated hydraulic conductivity given by Graham et. al., (1997) as \(5.0 \times 10^{-13} \text{ m/s}\) was converted to its
corresponding intrinsic permeability. Based on this approach, its air entry value was
determined as 0.7 MPa, thus yielding a water retention curve shown in Figure 5.7.

The approach proposed by Gens et al., (1998) was adopted to determine the hydraulic
conductivity relationship for granite;

\[ k_l = k_{sat} \times S_i^{1/2} \left( 1 - \left( S_i^{1/2} \right)^2 \right) \text{ m/s for } S_i \leq 1 \]  

(5.8)

where \( k_{sat} \) is the saturated hydraulic conductivity equal to \( 5.0 \times 10^{-13} \) m/s (Graham et al., 1997), and \( k_l \) is the hydraulic conductivity. The relationship is shown in Figure 5.8.

The thermal conductivity for the granite is taken at a constant value of 3.6 W/m/K
(Graham et al., 1997). The specific heat capacity for the rock, \( C_{psoil} \) was measured as
1060 J/kg.K (Graham et al., 1997).

5.2.2.2 Mechanical material parameters

For the analysis, the granite rock was assumed to deform elastically. As such, only
mechanical parameters defining the linear elastic behaviour of the rock are described
in this section.

Graham et al., (1997) gave Young’s modulus, \( E \), for the granite as 60 GPa, and
Poisson’s ratio, \( \nu \), as 0.22. Young’s modulus can be expressed in terms of the bulk
modulus, \( K \), and shear modulus, \( G \), by the following expression;

\[ E = \frac{9KG}{3K + G} \]  

(5.9)

and that Poisson’s ratio may be expressed as;

\[ \nu = \frac{3K - 2G}{6K + 2G} \]  

(5.10)

the following values were derived for the shear modulus and the bulk modulus
respectively; \( G = 17.9 \) GPa, and \( K = 26.0 \) GPa.
As it was anticipated that deformation caused by changes in suction within the rock would be insignificant, the elastic stiffness parameter for changes in soil suction, \( k_s \), was set to a negligible value.

### 5.2.3 Backfill material parameters

Due to a lack of information on the material parameters for the backfill material used in the experiment, alternative well defined material datasets have been identified which closely, as possible, match the behaviour of the backfill. The buffer used in the Buffer/Container Experiment is a 50:50 sand/clay mixture, whilst the backfill material is a 75:25 sand/clay mixture. It was therefore assumed reasonable to adopt (where necessary) the material parameters used for the sand/bentonite buffer.

#### 5.2.3.1 Thermal/hydraulic/mechanical parameters

In the Buffer/Container Experiment, the backfill had an initial maximum dry density of 2.13 Mg/m\(^3\) and an initial water content of 7.2 % (Graham et al., 1997). This affects both the water retention curve and the hydraulic conductivity relationship. The thermal conductivity relationship was assumed to be similar to the buffer material. Using experimental data obtained from Wan et al., (1995), a curve was fitted to the data (as shown earlier in Figure 5.1). The curve is graphically represented in Figure 5.9 and may be defined by the following equations:

\[
S_r = 1 + 7.0 \times 10^{-9} \left(1 - \exp\left(6.5 \times 10^{-6} \times s\right)\right) \quad s < 2.36 \text{ MPa} \quad (5.11)
\]

\[
S_r = -0.595 \log_{10}(s) + 4.75 \quad 2.36 \text{ MPa} < s < 14.83 \text{ MPa} \quad (5.12)
\]

\[
S_r = -0.308 \log_{10}(s) + 2.69 \quad 14.83 \text{ MPa} < s \quad (5.13)
\]

The unsaturated hydraulic conductivity curve was determined using the approach proposed by Green and Corey (1971) using a measured saturated hydraulic conductivity of \( 1.0 \times 10^{10} \) m/s (Graham et al., 1997). The variation of the unsaturated hydraulic conductivity with degree of saturation is shown in Figure 5.10. The relationship was applied in the finite element code COMPASS as a series of data points with linear interpolation used between the discrete values.
There was little information available to the author on the mechanical behaviour of the backfill material. Hence, the mechanical material parameters used for the sand/bentonite buffer have been adopted in the analysis of the backfill.

5.2.4 Sand material parameters

A layer of sand annulus was placed around the heater to protect the buffer from the heat during compaction in the borehole. Initially, a 100 mm thick layer of dry sand was placed at the bottom of the borehole to support the heater. The placement of the heater was conducted with great care so that a 50 mm uniform sand annulus was achieved around it. Finally a 300 mm thick layer of sand was placed above the heater. The sand annulus' density was taken as measured at 1.70 Mg/m$^3$ (Graham et al., 1997). The particle size distribution for the sand was found to be similar with those of Garside Grade medium sand, which has been well characterised (Ewen and Thomas, 1987). Hence, the material parameters for the Garside Grade medium sand have been taken for the sand annulus and used in the modelling work for the Buffer/Container Experiment.

5.2.4.1 Thermo/hydraulic parameters

The water retention curve proposed by Ewen and Thomas (1987) for the Garside sand has been adopted for the sand annulus in the Buffer/Container Experiment and is presented as follows:

$$ S_r = \left( \frac{s}{2.000} - 1181.8 \right)^{-0.75} + 0.0025 $$

s > 2430 Pa  \hspace{1cm} (5.14)

$$ S_r = \left[ \frac{\left( s \rho_w \right)^{0.0226249}}{1.101416 \times 10^{-26}} + \theta - 0.0025 \right] $$

s < 2430 Pa  \hspace{1cm} (5.15)

where $\rho_w$ in terms of kg/m$^3$, represents the density of water; the porosity of the sand, $\theta$, was taken as 0.302. The water retention curve is graphically represented in Figure 5.11.
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The thermal conductivity for sand was measured at 1.5 W/m/K and the hydraulic conductivity to be $6.25 \times 10^{-5}$ m/s (Mitchell, 2002). The sand was assumed to be an undeformable rigid material, and therefore no mechanical parameters were required.

5.2.5 Concrete

Concrete was put in place to restrain the backfill from swelling and to prevent moisture from escaping out into the room. As there was a lack of experimental data on the hydraulic and flow behaviour of the concrete, the author has adopted the water retention curve and hydraulic conductivity relationship proposed for the granite in place for the concrete. The dry density for the concrete was 2430 kg/m$^3$. The thermal conductivity was measured at 1.8 W/m/K, and the specific heat capacity was measured at 900 J/kg/K (Graham et al., 1997).

There was also little information available on the mechanical behaviour of the concrete. As such, the mechanical parameters used for the granite rock have been adopted in the deformation analysis of the concrete.

5.3 In Room Emplacement

The In Room Emplacement geometry was proposed by AECL as a potential design concept for a horizontal canister deposition configuration. Hence it is only possible at this stage to assume the required material parameters to be based on available datasets for alternative similar materials.

The following sections describe the flow and deformation parameters applied for the materials proposed in the In Room Emplacement.

5.3.1 Inner buffer

The inner buffer is to consist of 100% bentonite (AECL, 2002). A review showed that MX-80 Bentonite is also 100% bentonite, and is well defined (Borgesson et al., 1996). Personal communication with AECL (2002) indicated that where appropriate, material relationships developed for MX-80 Bentonite may be adapted for the analysis.
5.3.1.1 Thermo/hydraulic parameters

AECL (2002) proposed a thermal conductivity relationship for the inner buffer. The relationship is shown in Figure 5.12, and may be represented by the following set of equations:

\[ \lambda = 0.3 \text{ W/m/K} \quad S_f < 20\% \quad (5.16) \]

\[ \lambda = 1.583 S_f - 0.0167 \text{ W/m/K} \quad 20\% < S_f < 80\% \quad (5.17) \]

\[ \lambda = 1.25 \text{ W/m/K} \quad 80\% < S_f \quad (5.18) \]

AECL (2002) also provided information on the probable initial conditions of the inner buffer. The specific heat capacity, \( C_{p,\text{soil}} \) and the thermal expansion coefficient for the buffer were taken as 1290 J/kg.K and 2.3 x 10^{-4}/K respectively. The as-placed density for the inner buffer was taken as 1840 kg/m^3. After compaction, the initial porosity was thought to be 0.41, with an initial degree of saturation of 60%.

Research performed by Borgesson et al., (1996) found that a cubic form of relationship best represented the hydraulic conductivity relationship for unsaturated bentonite clay. The relationship has been adopted in the analysis and is shown as follows:

\[ K_i = (S_r)^2 K_{sat} \quad (5.19) \]

where \( K_i \) is associated with the hydraulic conductivity of saturated clay, \( K_{sat} \) and the degree of saturation, \( S_r \). The saturated hydraulic conductivity of the inner buffer in freshwater and saline conditions were suggested as 5.0 x 10^{-13} m/s (AECL, 2002). Figure 5.13 shows the relationship between hydraulic conductivity and degree of saturation for the inner buffer.

Using data obtained from Borgesson et al., (1996) and adopting the van Genuchten (1980) approach, a mathematical expression which gave the closest fit to the data was derived. The correlation between suction and degree of saturation for the inner buffer is presented in Figure 5.14 and the equation used is shown as follows:
where $\alpha = 4.5 \times 10^{-7}$, $b = 1.75$, $\theta_{\text{res}} = 0.0001$, $\theta_{\text{sat}} = 0.41$. Both $\alpha$ and $b$ are curve fitting parameters, $\theta_{\text{res}}$ represents the residual water content, and $\theta_{\text{sat}}$ represents the saturated water content.

### 5.3.1.2 Mechanical material parameters

As mentioned earlier, little is known about the mechanical behaviour for the inner buffer. Hence, the mechanical parameters measured for the MX-80 Bentonite was adopted for this analysis (Borgesson et al., 1996). The deformation parameters shown below have been used in the numerical model:

- $k = 0.0125$
- $k_s = 0.094$
- $G = 10$ MPa

### 5.3.2 Outer buffer material parameters

The outer buffer was proposed to consist of a 50:50 mixture (by dry weight) of sand and bentonite. The outer buffer has not been modelled previously, therefore would need to adopt datasets from alternative similar materials. The outer buffer material is expected to be similar in origin and consistency to the buffer material used in AECL’s Buffer/Container Experiment. This was well characterised by Graham et al., (1994). Personal communication with AECL (2002) suggested that the parameter dataset developed for the buffer material used in the Buffer/Container Experiment may be used for the outer buffer with a number of revisions. Therefore the complete set of parameters is repeated here.

### 5.3.2.1 Thermo/hydraulic parameters

AECL (2002) proposed a thermal conductivity relationship for the outer buffer. The relationship was adopted for the analysis and is shown in Figure 5.12;
\[ \lambda = 0.7 \text{ W/m/K} \quad S_t < 20\% \]  
\[ \lambda = 1.667 S_t - 0.367 \text{ W/m/K} \quad 20\% < S_t < 80\% \]  
\[ \lambda = 1.70 \text{ W/m/K} \quad 80\% < S_t \]  
\[(5.21)\]  
\[(5.22)\]  
\[(5.23)\]

AECL (2002) also indicated a probable initial condition for the inner buffer in the proposed geometry layout. The specific heat capacity, \(C_p\) and the as-placed density for the buffer were taken as 1350 J/kg.K and 1980 kg/m\(^3\). AECL (2002) also proposed the initial porosity and initial degree of saturation at 0.38 and 80\% respectively.

The unsaturated conductivity relationship was taken as that shown earlier in Equation 5.19. The saturated hydraulic conductivities for the outer buffer at freshwater and saline conditions were given as \(1.0 \times 10^{-12}\) m/s and \(1.0 \times 10^{-10}\) m/s respectively (AECL, 2002). Figure 5.15 presents the relationship between hydraulic conductivity and degree of saturation for the outer buffer.

Experimental data was obtained from Wan et al. (1995) and subsequently adjusted to match the initial porosity for the outer buffer. This produced a curve which relates suction to degree of saturation for the outer buffer. This is graphically represented in Figure 5.16 and may be defined using the following equations;

\[ S_r = 1 + 9.847 \times 10^{-6} [1 - \exp(3.67 \times 10^{-6} \times s)] \quad s < 2.20 \text{ MPa} \]  
\[ S_r = -0.58836 \times \log_{10}(s) + 4.70 \quad 2.20 \text{ MPa} < s < 14.83 \text{ MPa} \]  
\[ S_r = -0.308 \times \log_{10}(s) + 2.6895 \quad s > 14.83 \text{ MPa} \]  
\[(5.24)\]  
\[(5.25)\]  
\[(5.26)\]

The thermal and hydraulic parameters described above have been incorporated into the model for the analysis of the outer buffer.

### 5.3.2.2 Mechanical material parameters

The deformation behaviour of the outer buffer was assumed to be similar to the sand/bentonite buffer described earlier for the Buffer/Container Experiment. For a
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non-linear elastic model, the following principal data was taken from Mitchell (2002) and applied in the analysis for the outer buffer;

\[ \kappa = 0.0125 \]

\[ \kappa_s = 0.0111 \]

\[ G = 10 \text{ MPa} \]

5.3.3 Gap backfill

The gap backfill in the proposed In Room Emplacement consists of pelletized bentonite material. Similar to other materials found in the design layout, the gap backfill has not been modelled previously. AECL (2002) suggested that the parameters obtained for the MX-80 Bentonite can be assumed for the gap backfill. The following sections describe the flow and deformation parameters for the gap backfill.

5.3.3.1 Thermo/hydraulic parameters

AECL (2002) proposed a thermal conductivity relationship for the gap backfill. The proposed correlation between thermal conductivity and degree of saturation for the gap backfill is shown in Figure 5.17 and may be represented by the following equations;

\[ \lambda = 0.3 \text{ W/m/K} \quad S_I < 20 \% \quad (5.27) \]

\[ \lambda = 1.5 \times S_I \text{ W/m/K} \quad 20 \% < S_I < 80 \% \quad (5.28) \]

\[ \lambda = 1.2 \text{ W/m/K} \quad 80 \% < S_I \quad (5.29) \]

The specific heat capacity, \( C_{\text{psoil}} \) and the as-placed density for the gap backfill were taken as 910 J/kg.K and 1410 kg/m\(^3\) (AECL, 2002). Furthermore, the initial porosity was proposed at 0.49, and the initial degree of saturation at 6 %.

As there was little information on the unsaturated hydraulic conductivity, the cubic form of flow relationship proposed for the inner buffer was adopted for the gap backfill. The saturated hydraulic conductivities at freshwater and saline conditions of
the gap backfill were assumed as $1.0 \times 10^{12}$ m/s and $1.0 \times 10^{12}$ m/s respectively (AECL, 2002). Figure 5.17 plots the hydraulic conductivity against degree of saturation for the gap backfill. As there were no available datasets on the suction behaviour of the gap backfill, the water retention curve proposed for the outer buffer was adopted.

5.3.3.2 Mechanical material parameters

The principal deformation parameter adopted for the gap backfill was assumed from the relationship proposed for the outer buffer;

$$\kappa = 0.0125$$

$$\kappa_s = 0.011$$

$$G = 10 \text{ MPa}$$

5.3.4 Dense backfill

For the In Room Emplacement, the dense backfill was proposed by AECL (2002) to be a mixture of bentonite clay, lake clay and aggregate at a dry weight composition of 5:25:70. The dense backfill has not been modelled previously and would need to assume parameters defined for other similar materials. Personal communication with AECL (2002) suggested that parameters developed for the backfill material in the Buffer/Container Experiment may be assumed where required.

5.3.4.1 Thermo/hydraulic parameters

A thermal conductivity relationship was proposed for the dense backfill material (AECL, 2002). The relationship is shown in Figure 5.12 and may be represented by the following set of equations;

$$\lambda = 1.0 \text{ W/m/K} \quad S_i < 20 \% \quad (5.30)$$

$$\lambda = 1.667 S_i + 0.667 \text{ W/m/K} \quad 20 \% < S_i < 80 \% \quad (5.31)$$

$$\lambda = 2.0 \text{ W/m/K} \quad 80 \% < S_i \quad (5.32)$$
The specific heat capacity, $C_{ps0ii}$, and the as-placed density for the dense backfill were taken as 1100 J/kg.K and 2280 kg/m$^3$ (AECL, 2002). The initial porosity was given as 0.22, and the initial degree of saturation was taken as 80%.

The saturated hydraulic conductivity of the dense backfill at freshwater and saline conditions was assumed as $2.0 \times 10^{-11}$ m/s (AECL, 2002). The hydraulic conductivity relationship shown earlier in Equation 5.19 was adopted for the dense backfill. The correlation between hydraulic conductivity and degree of saturation for the dense backfill is shown in Figure 5.19.

The backfill material defined in the Buffer/Container Experiment was well defined and its hydraulic parameters can be assumed for the dense backfill. Experimental data presented by Wan et al., (1995) was adopted and adjusted to match the initial porosity for the dense backfill. Applying the van Genuchten (1980) equation (described earlier in Equation 5.20), a mathematical expression that closely matched the retention curve was derived, where $\alpha = 2.2 \times 10^{-11}$ m/s, $b = 1.8$, $\theta_{res} = 1.0 \times 10^{-4}$, and $\theta_{sat} = 0.22$. The resulting water retention curve is shown in Figure 5.20.

5.3.4.2 Mechanical material parameters

In order to model the mechanical behaviour of the dense backfill, a non-linear elastic model was used. The following assumed data has been used for this model:

- $\kappa = 0.01$
- $\kappa_s = 0.01$
- $G = 10$ MPa

5.3.5 Light backfill

The proposed material composition for the light backfill consists of a mixture of bentonite and sand at a dry weight composition of 50:50. As with other emplaced materials, the light backfill has not been modelled. Hence, some assumptions were required to establish the thermo/hydro/mechanical parameters for the theoretical model. AECL (2002) has suggested that where necessary, datasets from the
sand/bentonite buffer in the Buffer/Container Experiment may be assumed for the light backfill.

5.3.5.1 Thermo/hydraulic parameters

AECL (2002) proposed a thermal conductivity relationship for the light backfill material. The relationship is shown in Figure 5.12 and may be defined by the following set of equations;

\[
\begin{align*}
\lambda &= 0.5 \text{ W/m/K} \quad S_t < 20 \% \\
\lambda &= 1.5 S_t + 0.2 \text{ W/m/K} \quad 20 \% < S_t < 80 \% \\
\lambda &= 1.4 \text{ W/m/K} \quad 80 \% < S_t
\end{align*}
\]  

(5.33)  

(5.34)  

(5.35)

The specific heat capacity, \( C_{\text{psoil}} \) and the as-placed density for the dense backfill were taken as 1280 J/kg\cdot K and 1400 kg/m\(^3\) (AECL, 2002). It was also suggested that the initial porosity be taken as 0.55, and the initial degree of saturation be taken as 33 %. The proposed initial conditions have been adopted in the analysis of the light backfill.

AECL (2002) proposed the saturated hydraulic conductivity of the light backfill at freshwater and saline conditions as \( 1.0 \times 10^{-11} \) m/s and \( 1.0 \times 10^{-9} \) m/s respectively. The cubic form of hydraulic conductivity relationship (shown earlier in Equation 5.19) was adopted for the light backfill, and is presented in Figure 5.21.

Similarly for the outer buffer, experimental data from Wan et al., (1995) was assumed and adjusted to the initial porosity for the light backfill. The van Genuchten (1980) relationship was again employed to produce the best curve fit, which gave the graph fitting parameters \( \alpha \) and \( b \) as \( 4.0 \times 10^{6} \) and 1.8, and \( \theta_{\text{sat}} \) as 0.55. The suction against degree of saturation profile of the light backfill is shown in Figure 5.22.

The thermal and hydraulic parameters described above have been included in the model for the analysis of the light backfill.
5.3.5.2 Mechanical material parameters

In order to model the mechanical behaviour of the light backfill, the following assumed data has been used for this model:

\[ \kappa = 0.01 \]
\[ \kappa_s = 0.01 \]
\[ G = 10 \text{ MPa} \]

5.3.6 Granite rock material parameters

Similar to the emplaced materials, the granite rock has yet been characterized. However, it is likely that the In Room Emplacement would take place in AECL's Underground Research Laboratory (URL), situated in the Lac du Bonnet granite batholiths. As described earlier, Mitchell (2002) had conducted a review and defined the material relationships for granite rock in the Buffer/Container Experiment. Hence, the material relationships described for granite rock in the Buffer/Container Experiment were assumed similar to the granite rock in the In Room Emplacement.

In this section, the thermo/hydro/mechanical behaviour for the excavation damaged zones (EDZ) is described. The inner and outer EDZ layers represent 0.3 m and 1.0 m layer thick of rock away from the excavated surface of the In Room Repository.

5.3.6.1 Thermo/hydraulic parameters

The thermal conductivity for the rock was taken as 3.0 W/m.K, and the heat capacity was assumed as 845 J/kg.K (AECL, 2002).

As mentioned earlier, the granite rock material parameters for the Buffer/Container Experiment and the In Room Emplacement are assumed to be similar. Hence, adopting the relationship described in Equation 5.7 and using the experimental results presented by Davies (1991) in Figure 5.6, the threshold pressure can be determined for various regions in the granite rock, where:

Far field granite (1.3 m away from excavation and beyond) \( P_0 = 1.3 \text{ MPa} \)

Outer EDZ (0.3 m up to 1.3 m from excavation) \( P_0 = 1.2 \text{ MPa} \)
Inner EDZ (up to 0.3 m from excavation) \( P_0 = 0.4 \) MPa

Figure 5.23 presents the corresponding water retention curve based on the threshold pressure assumed for these regions of rocks.

The approach presented by Gens et al., (1998) was adopted for the granite rock in the In Room analysis. The proposed saturated hydraulic conductivity values for the inner EDZ, outer EDZ and far field rock were \( 1.0 \times 10^{10} \) m/s, \( 1.0 \times 10^{11} \) m/s and \( 1.0 \times 10^{12} \) m/s respectively (AECL, 2002). Equation 5.8 was subsequently used to produce a set of hydraulic conductivity curves for these rock regions, as shown in Figure 5.24.

The initial degree of saturation was varied according to the distance of the rock away from the excavated site. AECL (2002) proposed that at the far-field rock, initial porosity was 0.003 and fully saturated. At the outer EDZ, porosity remain unchanged but the degree of saturation was reduced to 50 \%. At the inner EDZ, the porosity was proposed as 0.006 and the degree of saturation at 20 \%. These recommendations have been included in the model for the analysis of the granite rocks.

### 5.3.6.2 Mechanical material parameters

Both inner and outer EDZ were assumed to have similar mechanical parameters as the granite rock. As described earlier, there was little information available on the mechanical behaviour of the granite rock. Hence, parameters for the granite rock were assumed to take after the material relationships (described earlier in Section 5.2.2) presented for the granite rock in the Buffer/Container Experiment.

### 5.3.7 Concrete

The concrete material in the In Room Emplacement consists of low-heat high-performance concrete (LHHPC). The concrete in the proposed layout has not been modelled previously. Hence, as a first approximation AECL (2002) acknowledged that it was acceptable to adopt the material relationships described for the granite rock in place for the concrete material.

### 5.3.7.1 Thermo/hydraulic material parameters

AECL (2002) suggested that the thermal conductivity and heat capacity for the concrete can be taken as 1.85 W/m.K and 900 J/kg.K respectively. These suggestions
have been included in the model. They also recommended the initial porosity for the concrete as 0.15. However, the porosity suggested for the concrete was based on the concept of ‘total’ porosity. AECL (2002) believed that “the porosity available for mass transport is likely to be discernibly lower due to occluded/isolated pore spaces within the concrete”. As such, the porosity was reduced to 0.003, similar to that used for the granite rock.

The hydraulic conductivity relationship proposed earlier for the granite rock has been adopted for the concrete. The saturated hydraulic conductivity in the concrete was suggested at $1.0 \times 10^{-12}$ m/s (AECL, 2002). The relationship for suction against degree of saturation proposed for the granite rock was also adopted for the concrete.

The thermal and hydraulic parameters have been included in the model to analyse the concrete in the proposed In Room layout.

5.3.7.2 Mechanical material parameters

Similar to the granite rocks, the mechanical behaviour for concrete has not been modelled previously. Hence, for the deformation analysis, the mechanical parameters described for the granite rock in the Buffer/Container Experiment have been adopted for the concrete section.

5.3.8 Copper Container

For the In Room Emplacement, AECL proposed using a copper container to store waste materials. Since the container was assumed to be impermeable and no deformation was expected, only the thermal parameters shall be described in this section.

AECL (2002) has suggested the thermal conductivity and heat capacity of the copper be taken as 380 W/m.K and 390 J/kg.K respectively. The copper density was assumed at 8930 kg/m$^3$. The above recommendations have been incorporated in the model for the analysis of the copper container.
5.4 Conclusions

The thermo/hydro/mechanical parameters required to model the Buffer/Container Experiment and the In Room Emplacement have been presented and described in this chapter. Where possible the parameters used have been obtained from laboratory test results or in situ testing of materials reported in the literature. However, this was not possible for every material, and where necessary, approximations have been made. A summary of the thermo/hydro/mechanical material parameters for AECL's Buffer/Container Experiment is given in Table 5.2. A summary of the thermo/hydro/mechanical material parameters for the proposed In Room Emplacement is presented in Table 5.3.

5.5 References


### Table 5.1 Chemical composition of the granite groundwater at AECL’s underground research laboratory

<table>
<thead>
<tr>
<th>Ion/parameter</th>
<th>Na$^+$</th>
<th>K$^+$</th>
<th>Mg$^{2+}$</th>
<th>Ca$^{2+}$</th>
<th>Cl$^-$</th>
<th>SO$_4^{2-}$</th>
<th>CO$_3^{2-}$</th>
<th>pH</th>
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</thead>
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<tr>
<td>meq/litre</td>
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<td>0.06</td>
<td>0.46</td>
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<td>1.12</td>
<td>3.5</td>
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<td>Material parameter</td>
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<td>Backfill</td>
<td>Sand</td>
<td>Concrete</td>
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<tr>
<td>-------------------------------</td>
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</tr>
<tr>
<td>Water retention curve (Pa)</td>
<td>Equations (5.1), (5.2), and (5.3) Figure 5.2</td>
<td>Equation (5.7) Figure 5.7</td>
<td>Equation (5.11), (5.12), and (5.13) Figure 5.9</td>
<td>Equations (5.14) and (5.15) Figure 5.11</td>
<td>Equation (5.7) Figure 5.7</td>
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<td></td>
</tr>
<tr>
<td>Hydraulic conductivity (m/s)</td>
<td>Figure 5.3</td>
<td>Equations (5.8) Figure 5.8</td>
<td>Figure 5.10</td>
<td>6.25 x 10^{-3} m/s</td>
<td>Equation (5.8) Figure 5.8</td>
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<td>3.6 W/m/K</td>
<td>Equations (5.4), (5.5), and (5.6) Figure 5.4</td>
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<tr>
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<td>1400</td>
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<tr>
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<td>N/A</td>
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Table 5.2 Summary of the thermo/hydro/mechanical material parameters used to model AECL's Buffer/Container Experiment
<table>
<thead>
<tr>
<th>Material parameter</th>
<th>Inner Buffer</th>
<th>Outer Buffer</th>
<th>Gap Backfill</th>
<th>Dense Backfill</th>
<th>Light Backfill</th>
<th>Granite Rock</th>
<th>Concrete</th>
<th>Copper Container</th>
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</thead>
<tbody>
<tr>
<td>Water retention curve (Pa)</td>
<td>Equation (5.20), Figure 5.14</td>
<td>Equation (5.24), (5.25) and (5.26), Figure 5.16</td>
<td>Equation (5.24), (5.25) and (5.26), Figure 5.16</td>
<td>Equation (5.20), Figure 5.20</td>
<td>Equation (5.20), Figure 5.22</td>
<td>Figure 5.23</td>
<td>Figure 5.23</td>
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<td>Equation (5.19), Figure 5.15</td>
<td>Figure 5.17</td>
<td>Figure 5.19</td>
<td>Equation (5.19), Figure 5.21</td>
<td>Figure 5.24</td>
<td>Figure 5.24</td>
<td>N/A</td>
</tr>
<tr>
<td>Thermal conductivity (W/m/K)</td>
<td>Equation (5.16), (5.17) and (5.18), Figure 5.12</td>
<td>Equation (5.21), (5.22) and (5.23), Figure 5.12</td>
<td>Equation (5.27), (5.28) and (5.29), Figure 5.17</td>
<td>Equation (5.30), (5.31) and (5.32), Figure 5.12</td>
<td>Equation (5.33), (5.34) and (5.35), Figure 5.12</td>
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<td>3.0</td>
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<tr>
<td>Specific heat capacity (J/kg/K)</td>
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<td>1100</td>
<td>1280</td>
<td>845</td>
<td>900</td>
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<td>17900</td>
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</table>

Table 5.3 Summary of the thermo/hydro/mechanical material parameters used to model AECL's In Room Emplacement
Figure 5.1  Soil – water retention curves of suction versus water content for the bentonite-sand buffer (Wan et al., 1995)
Figure 5.2  Water Retention curve for sand/bentonite buffer in the Buffer/Container Experiment
Figure 5.3  Hydraulic conductivity relationship for sand:bentonite buffer in Buffer / Container Experiment
Figure 5.4  Thermal conductivity against gravimetric water content for the sand/bentonite buffer (Graham et al., 1997)
Figure 5.5  Thermal conductivity relationship for sand/bentonite buffer in the Buffer / Container Experiment
Figure 5.6  Plot of threshold pressure *versus* intrinsic permeability for a wide variety of geologic material over a 13 order-of-magnitude range in intrinsic permeability (Davies, 1991)
Figure 5.7 Water Retention curve for granite rock with a threshold pressure (Po) of 0.7 MPa
Figure 5.8  Hydraulic conductivity relationship for the granite rock in the Buffer/Container Experiment
Figure 5.9 Water retention curve for the backfill used in the Buffer/Container Experiment
Figure 5.10 Hydraulic conductivity relationship for the backfill material in the Buffer/Container Experiment
Figure 5.11 Water retention curve for sand in the Buffer/Container Experiment
Figure 5.12  Thermal conductivity relationship for various emplaced materials in the In Room Emplacement
Figure 5.13 Hydraulic conductivity relationships for the inner buffer (100 % bentonite) in the in room repository
Figure 5.14 Water retention curve for the inner buffer (100% bentonite) in the In Room Emplacement
Figure 5.15  Hydraulic conductivity relationships for the outer buffer in the In Room Emplacement
Figure 5.16 Water retention curve for the outer buffer in the In Room Emplacement
Figure 5.17 Thermal conductivity relationship for gap backfill in the In Room Emplacement
Figure 5.18 Hydraulic conductivity relationship for gap backfill (100% bentonite pellets)
Figure 5.19 Hydraulic conductivity relationship for dense backfill material
Figure 5.20  Water retention curve for dense backfill material
Figure 5.21 Hydraulic conductivity relationship for light backfill
Figure 5.22  Water retention curve for light backfill in the in room emplacement
Figure 5.23 Water retention curve for various rock regions in the In Room Emplacement
Figure 5.24  Hydraulic conductivity relationship for various rock region in the In Room Emplacement
Chapter 6

Buffer/Container Experiment

6.1 Introduction

This chapter presents a full-scale thermo/hydro/mechanical analysis of the Buffer/Container Experiment. This includes several sensitivity analyses carried out by varying buffer permeability and the vapour diffusion flow law in the simulation of the experiment. As mentioned in Chapter 5, the Buffer/Container Experiment was performed by the Atomic Energy of Canada Limited (AECL). Essentially, this underground experiment sets out to examine the effects of heating on the performance of the dense sand-bentonite buffer that has been proposed for use in the Canadian Nuclear Fuel Waste Management Program. The experiment involved placing a 635 mm diameter, 2250 mm long heater in a 1240 mm diameter, 5000 mm deep borehole. The heater was surrounded by densely compacted bentonite-sand buffer material. The heater, representative of a container of nuclear fuel waste was introduced to represent the heat generated by the decay of the nuclear waste. The experiment was conducted below the floor of a room excavated at a depth of 240m in AECL’s underground research laboratory, located in Lac du Bonnet, Canada between 1991 and 1994. The buffer and the surrounding rock were extensively instrumented with a series of thermistors, packer strings, pressure transducers, displacement gauges and radial strain cells to monitor the transient changes of temperatures, total pressures, water pressures, suctions, and rock displacements.
Section 6.2 describes the experimental set-up adopted by AECL in their underground laboratory, and the distinct phases of the Buffer/Container Experiment. In Section 6.3, the experimental results describing the temperature field, the moisture field in the rock, the transient water content and suctions measured in the buffer, the pressure in the buffer, the displacements in the rock as well as the water contents measured during decommissioning are reported.

Section 6.4 presents the numerical simulation of the pre-heating phase. A thermal hydraulic simulation of the Buffer/Container Experiment when heating is initiated is presented in Section 6.5. In Section 6.6, the influence of swelling behaviour on moisture flow is investigated. Section 6.7 investigates further the influence of swelling behaviour on moisture flow and in particular looks at the effect of water storage within the micro-macro structure. Section 6.8 presents a coupled thermal hydraulic simulation that includes swelling effects on moisture flow and the rate of adsorption/desorption in the buffer material.

Section 6.9 details a coupled thermo/hydro/mechanical analysis of the heating phase, incorporating the influence of swelling phenomena discussed in Section 6.8. This is followed by Section 6.10 which investigates, via a sensitivity analysis, the effects of varying the buffer’s saturated hydraulic conductivity and key parameters in the vapour flow law.

Finally, Section 6.11 summarises the conclusions drawn from this work.

6.2 Experimental Set-up

The schematic layout of AECL’s concept for deep underground disposal of nuclear waste is presented in Figure 6.1. A series of boreholes would be drilled using high pressure water jets into the floors of underground caverns. Following that, the canisters would be placed into the drilled boreholes which were later backfilled with an engineered buffer material. Finally, the cavern and tunnel would be backfilled using a granite-clay mixture.

The Buffer/Container Experiment construction layout is based on AECL’s concept for deep geological waste disposal. Figure 6.2 - 6.4 present a detailed overview on
Chapter 6  Buffer/Container Experiment

the geometry of the experiment and positions of the recording instruments in the buffer and the rock. In the Buffer/Container Experiment, a heater representative of a canister containing radioactive waste was installed in a sand/bentonite buffer within a 1240 mm diameter, 5000 mm deep borehole. The experimental set up was installed at the 240 m level in AECL's underground research laboratory. Observing Figure 6.2, it can be seen that a 50 mm thick sand annulus surrounds the heater in the Buffer/Container Experiment. According to Dixon et al. (1993) the sand serves to protect the heater during compaction of the buffer and to reduce the amount of shrinkage expected during the heating period.

At the top of the buffer, a 1 m layer of backfill, a concrete cap, and a set of restraining columns propped against the roof of the experimental Room 213 were set in place to restrict the swelling and any moisture movements out or into the buffer. Extensive instrumentation was implemented prior to the placement of the buffer. These measuring devices were able to record measurements prior to the heater activation, during the heating period and during decommissioning. These experimental data would later be used to compare against the numerical results, shown later in this chapter.

As for the construction and experimental phases for the Buffer/Container Experiment, the excavation took place between June 1989 and September 1989. Excluding the excavation of the experimental room, the experiment had gone through six distinct stages; Phase A to Phase F. Table 6.1 presents the timing and duration for each phases and the nature of work that had taken place.

6.3 Experimental Results

The experiment results recorded using instrumentation placed in the buffer and the rocks have been presented in a report produced by Graham et al., (1997). In that report, the transient changes in temperature, pore water pressure and suction, deformation and stress were described. Results presented by Graham et al. (1997) are repeated here for readers to gain an understanding on the actual experimentations and results, as well as highlighting some of the findings made from the Buffer/Container Experiment.
6.3.1 Temperature Field

Before the excavation process began, the temperature in the granite rock was approximately 284 K. However, the construction of the tunnels and caverns in the surrounding area meant the temperature distribution was affected. According to Graham et al., (1997), air temperature within the tunnel varied between 285 K and 291 K prior to the heating phase of the experiment. The report also detailed the temperature distribution in the near field rock. At the beginning of Phase D (heating period), air heaters were installed to maintain the room air temperature at 288 K but had only limited success. Graham et al., (1997) suggested that the seasonal variations in the cavern temperature could be neglected as its influence was negligible compared to the influence of the heater.

The heater power was initially activated at a constant power of 1000 W but was increased to 1200W after 26 days of heating. The increase was necessary as the thermal conductivity of the sand was previously underestimated during the pre-experiment modelling exercises, which also meant that the target temperature of 358 K could not be reached within the experiment timescale. Following the increase in power, the skin temperature of the heater reached the target value after 126 days of operation. Figure 6.5 presents the experimental transient temperature profile along the mid-height of the heater. The temperature results are only presented up to 210 days as there was minimal change after that. Observing the temperature profile, a steep temperature gradient can be seen across the sand annulus and the buffer. The temperature gradient in the near field rock is less pronounced. The transient vertical temperature profiles through the emplacement borehole centre are shown in Figure 6.6. As only minimal changes in temperature were observed after 350 days, further results have not been shown here. The top layer of the buffer was in direct contact with the backfill, and the backfill was in direct contact with a concrete cap. Since the concrete top cap was exposed to the room temperature, this had a cooling effect on any temperature increase arising from the heating.

6.3.2 Moisture Field in the Granite Rock

The regional hydrostatic water pressure at 240 m depth was measured at 2.1 MPa (Chandler et al., 1992). It was suggested that excavation would have a draw down
effect on water pressures in the rock region close to the excavation. Accounting for the draw down of the water table due to construction of the underground caverns, an average far field pore water pressure of 1600 kPa was reported by Chandler et al., (1992).

Figure 6.7 illustrates the pore water pressure results at the end of Phase B and C (also known as the ‘dwell’ period) as recorded using hydraulic packers and piezometers. According to Graham et al., (1997) the hydraulic packers gave reliable readings except for the top cells in packer hole HG 7 (3.5 m from the centre of the borehole) and the lowest cell in packer HG 8 (2.5 m from the centre of the borehole). Although readings from HG 7 and HG 8 were included in the report, Graham et al., (1997) did not consider them reliable.

Table 6.2 lists the positions of the piezometers. Measurements taken following emplacement of the unsaturated buffer have shown the de-saturation of the rock occurring at a distance approximately 2.0m from the centre of the borehole. As piezometers cavitate when suction in the rock exceeds 100 kPa, the actual values were not displayed.

Figure 6.8 details the transient pore water pressure for the rock at a 4 m by 8 m domain. Figure 6.9 presents the pore water pressure profiles at varying depths in the granite rock. The label HG shown in Figure 6.9 refers to a hydraulic packer, and the labels RH and RP refer to the piezometers. Initially, the piezometers registered negative pore water pressure but later during the heating period, the water began to recharge. The experimental results indicate that maximum pore water pressure values were reached at the beginning of the heating period, and then dissipated slowly. In their report, Graham et al., (1997) suggested that the early pressure peaks were due to thermal expansion in the pore water in the rock. However, the pore water pressure was unable to equalize immediately due to the low hydraulic conductivity within the granite rock. As the heating experiment progressed, the pressure build up slowly dissipated and a balance was achieved between the potential arising from the temperature increase in the buffer material and the pore water pressure increase in the rock. In Figure 6.8, an isolated region of high pore water pressure in the buffer region was observed. It was thought to be due to faulty readings from two of the hydraulic
packers positioned in the high pore water pressure region. In Figure 6.9, packers HG 8 and HG 9 which registered unusual high pore water pressure values have been marked with an asterisk, indicating the possibility of the instruments being faulty.

It is worth mentioning that the hydraulic piezometers were positioned in a region of leucocratic granite. This type of granite has larger porosity than the fine-grain granite in which the hydraulic packers were located. Comparison between the readings recorded by the hydraulic packers and the piezometers show that the piezometers’ reading were generally lower (at same depth and radius). Graham et al., (1997) thought that the larger porosity granite (leucocratic) could explain the lower registered pore water pressure results. However, it should be noted that the amount of leucocratic granite was small surrounding the experiment.

6.3.3 Water content and suction measurements in the buffer

Activation of the heater was expected to drive away moisture in the buffer close to the heater. The thermal needles were placed at locations (as shown in Figure 6.3) to measure the water content close to the heater. For buffer region that were expected to hydrate, psychrometers were put in place to measure the values.

Based on the average water content in the buffer at time of placement and adopting the soil-water retention curve for the sand-bentonite buffer (shown in Figure 5.2), the average matric suction was taken as 4.0 MPa. By the end of the ‘dwell’ period the matric suction had reduced to 3.5 MPa. Figure 6.10 shows the transient pore water pressure results for the buffer as recorded by the thermal needles and psychrometers. It can be seen that high suctions was noticeable adjacent to the heater as the experiment progressed. The drying front can be seen moving towards the buffer-rock interface. Figure 6.11 illustrates the comparison between the end-of-test water content and the thermal needles results. Obvious differences especially in the region of buffer above the heater were observed. Hydration was recorded at the buffer-rock interface. The hydration process was thought to be a combined effect of moisture escaping from the heater to the rock and infiltration of moisture from the rock into the adjacent buffer material.
During the decommissioning phase, corrosions were discovered on the thermal needles. The accuracy of the measurements taken by these corroded needles was thought to be impaired and inaccurate. Graham et al., (1997) suggested that results taken after 525 days of heating are interpreted qualitatively and not quantitatively.

6.3.4 Stress and Strain Profile in the Buffer and the Backfill

Vertical and horizontal pressures in the buffer and the backfill were recorded using total pressure cells. Figure 6.12 shows the distribution of vertical and horizontal pressure in the buffer and backfill for the duration of the experiment. Observing the horizontal pressures in Figure 6.12, a good degree of axial symmetry was measured. At day 'zero', a non-uniform pressure distribution was obtained. As the buffer was compacted in layers, the initial pressure distribution was initiated by a release of stresses built up during the compaction effort. A large increase in the horizontal and vertical pressure profile were measured at the beginning of the heating phase. The pressure subsequently began to dissipate as the heating phase progressed. Graham et al., (1997) postulated that the thermal expansion was the main reason behind the initial increase in pore pressure. Besides that, an overall upward force was observed for the vertical pressures profile. An overall upward force was observed from the vertical pressures profile. It was thought that the swelling pressure was higher at the bottom of the borehole. The lower vertical pressure above the top of the heater was probably due to the existence of deformable material which allowed some of the stress build up to be relieved. Contrary to expectation, the maximum horizontal pressure was not recorded adjacent to the heater. It was postulated that the buffer adjacent to the granite could have expanded into the fissures in the rock, thus reducing the pressure build up.

6.3.5 Displacements in the rock and the concrete restraining cap

Borehole extensometers were installed on the floor of the experimental room adjacent to the emplacement hole to measure the vertical deformation. Measurements taken during the heating experiment show minimal displacements, with a maximum of 0.72 mm recorded (Graham et al., 1997). There was good correlation with the temperature measurements in the rock whereby the cooler parts of the rock (above
Drilling the emplacement borehole was thought to result in stress release from the rock. Radial strain cells were used in the Buffer/Container Experiment to measure the radial displacements taking place. Readings taken from these instruments showed large displacement after the heater activation, with values approaching steady state after 100 days. Observing the experimental set up shown in Figure 6.2 the Buffer/Container Experiment was capped by a stiff steel top cap and Neoprene gasket. Both steel cap and gasket would inhibit swelling in the clay and minimise moisture loss between the top of the backfill and the Experiment Room 213. Looking at Figure 6.2, the top cap was braced against the roof of the experimental room using steel columns which were strain gauged to provide estimates of the swelling pressure. The system was designed to withstand 3 MPa swelling pressure and 1 MPa hydraulic pressure. Readings from the strain gauges recorded a maximum pressure of 350 kPa. However, the results did not match the lower pressure recorded using total pressure cells 1FR 1 and 1FR 2. Graham et al., (1997) thought that the columns would have been affected by the air temperature changes in the experiment room, thus distorting the pressure readings.

### 6.3.6 Decommissioning

During the heating phase of the experiment, it was felt that the readings obtained from instruments such as moisture needles and psychrometers were giving good qualitative changes but not accurate readings. However, during decommissioning the end-of-test water contents and its corresponding degree of saturation were determined. This allowed comparisons against values measured by the psychrometers and thermal needles during the heating phase.

Figure 6.11 presents a comparison between the water contents interpreted from thermal needles and psychrometers for day 525, and the decommissioning water content measurements. Readings obtained for day 897 were not admitted as the needles had corroded towards the end of the experiment.
The decommissioning results indicate a large decrease in water content in the buffer surrounding the heater. The buffer adjacent to the rock exhibited hydration. Graham et al., (1997) believed that thermal induced movement and water inflow from rock were largely responsible for the end-of-test water content distribution. Comparing both sets of water content results, good correlation was obtained. The decommissioned result show more drying at the top of the heater. The increase in moisture content along the buffer/granite interface for the end-of-test results were also much higher.

Graham et al., (1997) suggested that it was more appropriate to place higher confidence in the direct end-of-test moisture content measurements due to the higher number of samples taken from the decommissioning. Although sample disturbance as well as other external factors could affect the accuracy of the decommissioning results, the margin of error was not expected to be significant.

Decommissioning also showed development of small cracks (less than 1mm) in the buffer. It was believed that the cracks were due to desiccation in hot regions close to the heater or to stress release during excavation of the experiments. Such radial cracks could potentially be seen as pathways for migration of groundwater towards and away from fuel waste containers.

6.3.7 **Summary of the experimental results**

The temperature field was thought to be well understood with steady state temperature achieved in the buffer after 150 days and in the rock after 300 days. The pore water pressure results indicate a huge increase at the beginning of the heating stage before dissipating away after day 400. It was postulated by Graham et al., (1997) the initial increase was due to the thermal expansion of the pore water in the rock. Large amount of drying was observed in the buffer adjacent to the heater, whereas buffer next to the rock saw an increase of water content.

No significant movement was recorded for the rock. Although readings taken from the strain gauge and total pressure cells show discrepancies, patterns observed were broadly similar. Although decommissioning revealed desiccation cracking in the
buffer, the cracks were found to be limited to the inner third of the buffer annulus and did not extend to the buffer-rock interface (Graham et al., 1997).

Observing measurements taken for temperatures, suction and deformation, a visible symmetrical shape was achieved. It was believed that the end-of-test water content results provided a more accurate representation than those obtained from the psychrometers and thermal needles.

6.4 Numerical Simulation of the pre-heating phases

An initial simulation on the Buffer/Container Experiment had previously been reported in Mitchell (2002). However for some material parameters, revised values were obtained from AECL which were thought to be more closely representative of the materials present (AECL, 2001). Therefore although the focus of this study is the investigation of the effects micro and macro structure in soil has on the heating phase, the complete Buffer/Container Experiment has been re-analysed here to ensure that these revisions are fully accounted for. The Buffer/Container Experiment has been simulated using COMPASS (as described in Chapter 4) and the material parameters used in the numerical model have been described in Chapter 5.

6.4.1 Thermal simulation to establish domain size and boundary conditions

Mitchell (2002) found that a 15m by 16m domain size to be sufficiently large such that its boundary conditions yielded negligible influence on the near field results. Although the differences in the material properties were not thought to affect the size of the domain required, the simulation was re-analysed and this domain was found to suitable. The mesh as developed by Mitchell (2002) has been adopted for the preheating phase simulations and is shown in Figure 6.13. The results of these simulations also show that the influence of the upper boundary on the near field conditions were negligible and that the Buffer/Container Experiment can be assumed as two dimensional and axisymmetric about the centre of the borehole.
6.4.2 Simulation of Phase A, B and C – preheating phases

Initially, an isothermal hydraulic analysis was undertaken. Temperature variations in the rock were not simulated as the temperature field was not expected to vary during the drilling process.

The construction of the underground repository and drilling of the emplacement resulted in an initial draw down of pore water pressures in the rock. A 15 m by 30 m finite element mesh (as shown in Figure 6.14) was used to perform the hydraulic analysis to simulate the initial draw down effect in the rock following construction.

The exposed cavern boundaries and boreholes were fixed at 0 MPa (atmospheric pressure). Although the cavern was 240 m below ground level, the far field boundary condition was fixed at an average of 1.6 MPa, varying with elevation. Following Chandler et al. (1992), the initial pore water pressure in the rock followed a similar variation and at a depth of 240 m was 1.6 MPa. Any boundaries not prescribed a fixed pore water pressure were taken as having a zero moisture flux normal to the boundary.

Phase A was simulated for 280 days where pore water pressures eventually reached steady state. The pore water pressures results after 280 days were applied as the initial conditions for the dwelling period (Phase B & C). Comparison was not made against the experimental data as the hydraulic packers were still unstable during the drilling process.

6.4.3 Phase B & C – installation of the buffer and backfill and a dwell period

A thermal-hydraulic analysis of Phases B and C has been undertaken. The mesh shown in Figure 6.13 was employed for the dwell period simulation. Investigations found that once the initial draw down in the pore water pressure had been accounted for, the influence of the upper boundary of the mesh shown in Figure 6.14 was negligible. The mesh could then be substantially reduced in size and subsequently speed up the numerical analysis.
As mentioned earlier, the initial pore water pressure in the rock was taken from the final simulated results for Phase A. The initial gravimetric moisture content of the buffer was 17.9 %. Referring to water retention curve for buffer shown in Chapter 5, the initial average suction in the buffer has been taken as 4.0 MPa. The construction of the tunnels and caverns had affected the temperature distribution in the granite rock. According to Graham et al. (1997) the room temperature within the tunnels varied between 285 K and 291 K, with an average of 288 K prior to the heating phase of the experiment. The temperature gradient from the experiment room into the rock was well-defined in the literature (Graham et al., 1997) and was taken as the initial temperature in the rocks.

Figure 6.15 shows the numerical results for the pore water pressure contour and the pore water pressure profile at mid-height of the heater. Figure 6.16 shows an image of the numerically measured suction profile in the buffer at the end of Phase B & C. The rock at mid-height of buffer had desaturated up to 2.8 m away from the centre of the borehole. This gave a reasonable correlation when compared with the experimental results measured in the hydraulic packer shown in Figure 6.7. No significant developments of the temperatures field from the initial condition were found.

6.5 Phase D – Heating Period (Thermo/Hydraulic simulation)

The mesh shown in Figure 6.13 and the time stepping scheme used for modelling the dwell period were adopted for the coupled thermal hydraulic analysis for Phase D. The initial pore water pressure and temperatures were taken from the simulated end results for the dwell period. As for the boundary conditions, the far field boundaries were fixed at their initial temperature and hydraulic conditions. The exposed cavern was fixed at zero pore water pressure and at room temperature (284 K). A time dependent heat flux was applied at the heater’s surface to simulate the heater’s performance. The heater flux was fixed at 1000 W for the first 25 days, and subsequently increased to 1200 W for the remaining days, reflecting the experimental pattern. The materials’ thermal and hydraulic relationships are as described in Chapter 5 and have been incorporated for the simulation. Any non-prescribed
boundaries were prescribed a condition of zero moisture and temperature flux normal to the boundary surface.

The following sections compare the results from the numerical simulations with those experimentally measured. The ability of the numerical model to predict the temperature, moisture and suction distributions in the buffer and the rock are also discussed.

### 6.5.1 Temperature results

A comparison between the transient numerical results and the experimentally measured results are presented in Figure 6.17 and 6.18. Figure 6.17 presents the transient comparison for a cross-section at the mid-height of the heater (approximately 3.0 m below the top of buffer). Although the heating period was for 897 days, the temperature results along this cross-section are presented only up to 210 days as this was the last set of experimental results presented by Graham et al., (1997). They found that the temperatures had already peaked and demonstrated negligible change after 210 days; this was reflected in the numerical results. Overall, a good correlation was achieved with the experimental results. Looking at Figure 6.17, a change in temperature gradient was observed at the materials' interfaces (e.g. from the sand layer to the buffer layer). This was expected as each material's thermal conductivity relationship is different. The transient temperature profile along the centre of the emplacement borehole is illustrated in Figure 6.18. The numerical results gave excellent correlation when compared with the experimental results for the thermal field.

### 6.5.2 Moisture Field in the granite rock

The contour plots of pore water pressure for the near field granite rock at various periods in Phase D are shown in Figure 6.19. The simulation results show minimal changes in pore water pressure over time. However, at closer inspection the pressure was increasing gradually throughout the heating phase. On face value the numerically simulated results did not appear to correlate well with the experimental contour plots. However, it should be noted that the experimental plots were strongly influenced by two hydraulic packers, labelled as HG 8 and HG9 at the depths of −3.5 m and −5.6 m,
which registered unusually high pore water pressures. Figure 6.20 shows the experimentally measured pore water pressures for packers HG 8 and HG9 at various depths. It can be observed that packers at depth of 1 m and 1.4 m showed smooth curves. However, packers at depths of 3.5 m and 5.6 m were registering fluctuating measurements and appeared to be unstable throughout the experiment thus casting doubt over the measurements.

The transient pore water pressure profiles in the rock at various heights are illustrated in Figure 6.21. As mentioned earlier, RH and RP denote the hydraulic piezometers, whilst HG denotes the hydraulic packers. It is worth repeating here that the hydraulic piezometers cavitate when pore water pressure exceeds suction at a value equivalent to 100 kPa. As such the piezometers are unable to record high suction values. The asterisks marking HG 8 and HG 9 in Figure 6.21 indicate these instruments were giving questionable readings as suggested by Graham et al., (1997). At 1.4 m below the top of buffer, good agreement with the experimental result was achieved. However, the numerical result indicates that steady state had been reached as little changes were observed. At 3.0 m below the top of buffer, reasonable agreement was achieved although it was noted that the numerical results were higher than the experiment result in the rock region. At depth of 3.5 m from the top of buffer, the numerical simulation predicted a lower pressure than those measured in the packers.

It can be seen that the experimental pore water pressure profile peaked early in the experiment before dissipating thereafter. However this trend has not repeated in the simulation. Initially, Graham and his workers (1997) thought that this initial peak in the pore water pressures could have been triggered by the thermal expansion in the granite groundwater. Some preliminary numerical investigations by Mitchell (2002) indicated that thermal expansion would not explain such phenomena. As such this hypothesis was not investigated further by the author.

**6.5.3 Suction measurements in the buffer**

Figure 6.22 shows the comparison between the numerical and the experimental pore water pressure contours at day 60, day 150 and day 525 respectively. Reasonable agreement can be observed when comparing the numerical result with the experimental result. However, it can be seen that the buffer near the heater was much
drier in the experimental results. At day 525 in the simulation, the buffer close to the heater can be seen to be wetting. This is in contrast to the experimental plots which indicate that the same buffer region was showing no signs of the drying effect abating.

Overall, reasonable correlations were observed for the numerical results. It is possible that swelling in the microstructure was taking place near the buffer granite interface and resulting in a reduction in conductivity. However the applied hydraulic conductivity relationship proposed by Green and Corey (1971) is unable to capture this effect. Swelling in the buffer near the granite rock is thought to be restricting the flow of water from the granite to the buffer, thus causing the drying process to continue in the buffer near the heater. Thomas et al., (2003) simulated AECL’s Isothermal Experiment and found that an exponential hydraulic conductivity relationship provided closest approximation to the swelling phenomena observed in the buffer. Such an approach may also be valid in this case.

6.6 Phase D – Heating Period (Thermo/Hydraulic simulation including the swelling effect in the buffer)

6.6.1 Introduction

As mentioned above, it was possible that the swelling mechanisms could be affecting the hydraulic response in the buffer and the rock. As a first approach to investigate this, the exponential form of hydraulic conductivity relationship, as presented in Thomas et al., (2003) was applied to the numerical model. Research into available literature on the micro-macro structure in swelling clay shows that at a microscopic level, water in between clay layers influences the soil’s macroscopic behaviour such as the ability for water to flow. Pusch et al., (1990) reported that bentonite clays are made of stacks of flakes separated by adsorbed water.

The author believes that it is important to distinguish the difference between ‘adsorbed water’ and ‘absorbed water’. According to the Oxford Dictionary (1999), adsorb is defined as “the holding of molecules of a gas, liquid, or solute as a thin film on surfaces outside or within the material”. On the other hand, absorb is defined
as "soaking up liquid or another substance or assimilating". When montmorillonitic clay such as bentonite is wetted, water is attracted onto the surface of clay layers and held by forces such as hydration and physico-chemical attraction. However, as soon as sufficient energy is provided, the bonding is weakened and the water becomes free again. Henceforth, water bonded to the clay shall be known as adsorbed water and water not influenced by any external forces is known as free water.

Figure 6.23 shows a schematic representation extracted from Thomas et al., (2003) which illustrates the conceptual model for the adsorbed and free water in bentonite clay at saturated and unsaturated conditions. In the Buffer/Container Experiment, the granite rock and the concrete cap prevent the buffer from expanding. It is postulated that as water entered the buffer from the surrounding host rock, the buffer began to swell and the micropores would be saturated. As the buffer was restrained, the total porosity of the buffer would stay constant but the ratio of the micro and macro porosities was thought to be changing. Pusch (1998) believed that the swelling of clay particles would reduce the size of macropores. As only free water found in macropores was available for flow, this means that the rate of moisture flow in the buffer reduces as the material approaches saturation.

As mentioned earlier, Mitchell (2002) reported that an exponential relationship between free water content and hydraulic conductivity was thought to provide the close approximation to the swelling phenomena observed in the buffer. The relationship is given as:

\[
k_{\text{swell}} = k \times [S_a + w_f \times S_f \left( \exp \left( \frac{1 - w_f}{M_f} S_f \right) \right)]
\]  

(6.1)

where \(w_f\) represents the percentage of free water, \(M_f\) represents a curve fitting factor that affects the curvature near to fully saturated state, \(k_{\text{swell}}\) represents the hydraulic conductivity for swelling clay. As for the free water content in the buffer, Pusch et al., (1990) presented a theoretical relationship between dry density and the content of adsorbed water. They stated that for sodium montmorillonite clay with a dry density of 1.76 Mg/m\(^3\) (as used in the Buffer/Container Experiment), 94% of the water present would be adsorbed. Mitchell (2002) assumed \(w_f\) as 6% and \(M_f\) arbitrarily as -100. The proposed relationship is illustrated in Figure 6.24. Compared with the
hydraulic conductivity relationship (Green and Corey, 1971) used in the earlier thermal hydraulic simulation approach where the hydraulic conductivity is highest at saturated condition, the exponential relationship shows the rate of flow reducing drastically as the clay nears saturation. The modified relationship has been included for the numerical analysis.

6.6.2 Effects of Temperature on the hydraulic conductivity

The rate of water movement is also influenced by viscosity. As the temperature increases, the viscosity of fluid reduces which allows fluid to move with greater ease. During the heating phase, the temperature increase in the buffer, rock, backfill and concrete is thought to reduce the level of viscosity and consequently increase the hydraulic conductivity. The author simulated a representative one dimensional strip along the mid-height of the buffer with and without including the temperature effects on viscosity. To describe the temperature effect on viscosity, the relationship proposed by Kaye and Laby (1973) that relates the dynamic viscosity of the liquid water with the absolute temperature (see Equation 3.14) was applied in the numerical model. When comparing both simulations, the simulation which considers temperature effect indicated lower suction in the buffer near the heater and lower peak temperature. The hydraulic conductivity increase has allowed groundwater to infiltrate more easily into the buffer, thus reducing both temperature rises and the drying effects in the buffer near the heater. As it became obvious that the heating was affecting the hydration process, the relationship proposed by Kaye and Laby (1973) was incorporated in the numerical model.

6.6.3 Numerical Challenges Encountered

Initial numerical simulations revealed a number of numerical analysis problems. The obstacles were identified and changes were subsequently introduced. The following section discusses one of the key difficulties encountered during the numerical simulation and how it has been resolved.

The mesh used previously for the heating phase (shown in Figure 6.13) was applied initially, incorporating the exponential hydraulic conductivity relationship for the buffer material, to simulate the heating period. However, the simulation was
unsuccessful. Oscillations were recorded in the buffer near the heater. Introduction of the exponential hydraulic conductivity relationship caused a standstill in the moisture flow as the buffer adjacent to the host rock was approaching saturation. Observing Figure 6.24 and Equation 6.1, hydraulic conductivity reduces to near zero as the buffer approaches saturated state. The sharp hydraulic gradient between the buffer material adjacent to the rock that is saturated but choked, and the buffer material near the heater with high suction value, poses great numerical difficulties for a numerical convergence. It was thought that to overcome this numerical challenge, the mesh needed to be discretized even further in the buffer and the near field rock.

The mesh used in the simulation was further discretized and shown in Figure 6.25. Numerical simulation performed for Phase D using the original hydraulic conductivity curve was repeated using the refined mesh and the results were compared with those presented earlier in Section 6.5. The differences were negligible and the mesh was adopted for future analysis that uses exponential form of hydraulic conductivity relationship.

6.6.4 Comparison between Numerical results and Experimental results

The numerical pore water pressure results in the buffer are shown in Figure 6.26 for comparison with the experimental pore water pressure contours. An improved correlation was obtained when compared with the results from earlier analysis using non-swelling buffer material parameters and relationships. In the experiment, less drying was observed above and below the heater after day 525 than was simulated. However it should be noted that the end-of-test moisture content results, presented in Figure 6.11, indicates almost equal amounts of drying being measured above and below the heater. The final measurements suggest that the buffer-granite interface is getting wetter whereas the buffer near the heater is drying. It was thought that the end-of-test results gave a better representation of the Buffer/Container Experiment at its final stage than those obtained from the thermal needles and the psychrometers (Graham et al., 1997).

As water began to infiltrate into the buffer material, the size of the micropores increased. However, as mentioned before, the buffer materials were restrained from expanding. As such, the macropores would reduce in size. Free water which is found
in macropores contributes to the hydraulic conductivity. As such, a decrease in macropores’ size would inhibit the flow of moisture. Using the exponential form of hydraulic conductivity relationship as a first attempt to capture the phenomena, it can be seen that the drying simulated near the heater was greater than using a non-swelling relationship.

The pore water pressure contour plots in the near field rock and the transient pore water pressure profiles in the rock at -1.4 m, -3.0 m and -3.5 m from the top of the buffer are displayed in figure 6.27 and 6.28. With the exception for the profile at -3.0 m, it can be seen that good correlations were measured when compared with the experimental results. Incorporating the choking effect into the simulation produced a higher pressure build up near the rock. As the buffer-granite interface becomes saturated and swells up, higher suctions and higher temperature in the buffer near the heater were simulated. The hydraulic gradient naturally draws water from the rock. However, as the hydraulic conductivity at the buffer-rock interface reduces greatly as it reaches saturation, pore water pressures in the rock begin to build up. Figure 6.27 shows the simulated results in the rock remaining unsaturated near the top of the Buffer/Container Experiment where it was in contact with the cavern. As the cavern was exposed, the recharge of the water table was slower as moisture evaporates into the cavern.

Figure 6.28 shows that the inclusion of the swelling effect in the buffer material produced a higher pressure build up than those recorded on the hydraulic piezometers. Graham and his workers (1997) believed that the hydraulic piezometers IRP2M to IRP5m were positioned in leucocratic granite, which was much coarser and would be expected to have a higher saturated hydraulic conductivity. This could result in the buffer material near these rocks being able to absorb moisture more readily, and the pore water pressures would need a longer time to recharge. Nevertheless, the author believes that the material difference in the rock could not explain satisfactory why the simulated pore water pressure in the rock was much higher than those observed from the experiment. Observing Figure 6.28, the simulated pore water pressure results at -1.4 m and -3.0 m from top of the buffer were higher than the experimental recordings. Although the swelling of the buffer has been simulated, the pore water pressure build up in the rock is far too high.
possible that the exponential form of the hydraulic relationship used in this analysis requires further investigation. It is postulated that instead of completely choking the flow of water in the buffer material when it is saturated, a lesser form of choking or retardation of water flow in the buffer may be occurring. The following section details an investigation of the exponential hydraulic relationship used to represent the effect of swelling in the buffer.

6.7 Phase D – Thermal/Hydraulic simulation: Investigation of the Relationship Representing Swelling Phenomena

6.7.1 Introduction

Although it has been demonstrated in Section 6.6 that the swelling hydraulic conductivity relationship presented by Mitchell (2002) has improved the correlation against the experimental results, the pore water pressure build up in the rock was overestimated. It was thought that instead of completely choking the flow of the water as the buffer becomes saturated, it is possible that the flow of water is only retarded or slowed down. As the high hydrostatic pressure from the rock infiltrates along the buffer-granite interface, the micropores becomes saturated, followed by the macropores. It is postulated that at saturated state, not all available water pathways have been blocked and free water is still able to flow, albeit in a much reduced quantity.

Revisiting the relationship presented in Equation 6.1, the term \(M_f\) effectively represents a curve-fitting factor that affects the curvature as the buffer approaches saturation. Although it is a non-measurable parameter, it acts to determine the level of influence the degree of saturation has on the ability of the free water to flow. Figure 6.29 illustrates various hydraulic conductivity curves with varying \(M_f\) values. It can be observed that as the \(M_f\) value reduces, the effect of swelling on conductivity reduces. Two different \(M_f\) values of 0.1 and 1.0 have been applied to investigate their potential to simulate the experiment by allowing some water to pass through saturated buffer elements. The simulated results are discussed and the correlations against the experiment results are shown the following section.
6.7.2 Comparison between Numerical Results and Experimental Results for Moisture Field in the Granite Rock and Suction in the Buffer Material

Figure 6.30 presents the simulated contour plots of pore water pressure for the near field granite rock at day 60, day 150 and day 525 using $M_f = 0.1$ and $M_f = 1.0$. The plots for $M_f = 100.0$ is presented in Figure 6.27. As $M_f$ was decreased from 100 to 0.1, the level of pressure build up in the near field rock was reduced. For example, while the plots for $M_f = 0.1$ indicate the near field rock remained unsaturated, plots for $M_f = 100.0$ that show the same region to be fully saturated with a high pressure build up.

Figure 6.31 presents the simulated pore water pressure contours for $M_f = 0.1$ and $M_f = 1.0$ in the buffer at day 60, day 150 and day 525 respectively. Comparison against measurements taken from psychrometers and thermal needles gave good correlation with the numerical results. For all three cases, the buffer next to the heater remained unsaturated even at day 525. This correlates well with the experimental plots where the drying effect becomes increasingly pronounced. The buffer region below the heater showed signs of wetting as water from the rock begins to infiltrate.

The transient pore water pressure profiles in the rock at -1.4 m, -3.0 m and -3.5 m from the top of the buffer for $M_f = 0.1$ and $M_f = 1.0$ are presented in Figure 6.32 and 6.33. The transient plots for $M_f = 100.0$ had been presented earlier in Figure 6.28. Observing the transient plots, a varying correlation with the measured experimental results can be seen. A gradual pressure build up in the rock was simulated in all three cases, with $M_f = 100.0$ giving the highest pressure increase. At 1.4 m below the top of buffer, the pore water pressure prediction in the rock was good for all three different $M_f$ values. At 3.0 m below the top of buffer, $M_f = 0.1$ provided better prediction than $M_f = 1.0$ and $M_f = 100.0$. At 3.5 m below the top of the buffer, all three cases overestimated the pore water pressure in the rock when compared with the measurements taken from the hydraulic packers and piezometers installed in the Buffer/Container Experiment. As mentioned previously, piezometers denoted HG8 and HG9 were thought to give suspicious readings.

Observing the numerical results obtained from the investigation of the swelling
phenomena in the Buffer/Container Experiment, it can be seen that the level of retardation applied onto the adsorbed water was affecting the resaturation process. Using a lower $M_f$ value has provided an improved correlation against the experimental results. In the analysis presented in Section 6.6, water was effectively choked as the buffer became saturated. However, instead of completely choking the flow system, the lowering of the $M_f$ parameter has permitted water to continue flowing through albeit at a slower rate. The rate of pressure build up became slower as the influence swelling has on the buffer was reduced.

6.7.3 Conclusions

The simulations that have different swelling relationships provide interesting results and indicate that the system is sensitive to the relationship used to represent swelling phenomena. However, it is believed that such adjustment of the relationship representing the choking effect in the buffer has not correctly captured the swelling phenomena. It was decided that further investigation into the transient nature of moisture movement between the micro and macro structure within the buffer was needed. The transient behaviour for the free water and adsorbed water under thermal effect during resaturation has therefore been examined in the next section.

6.8 Phase D – Thermo/Hydraulic Simulation including the Transient Effect of Free-Adsorbed Water

6.8.1 Introduction

As mentioned above, the contribution from the adsorbed water in the interlamellar space to the hydraulic conductivity in montmorillonitic clay is negligible. Hence, only free water found in the macropores and in between clay peds are available for flow. In the earlier simulations which used the swelling exponential hydraulic conductivity relationship, 94% of the moisture in the sand-bentonite material was assumed adsorbed and the remaining 6% as free water. However, it is believed that a fixed free and adsorbed water percentage is valid only when steady state is achieved in the clay-water system.

Observing the experimental results for the pore water pressure distribution in the rock
and the suction profile in the buffer from Figure 6.9 and Figure 6.10, a gradual pressure build up in the rock was recorded. In addition, the buffer near the rock remained wet whilst the buffer near the heater remained dry. It is postulated that not all water which filtered through the buffer-rock interface was adsorbed instantaneously. In other words, it is envisaged that a time-dependent relationship exists for the adsorption of free water (from the rock) in between the clay intralayers.

A scenario is now postulated for the in situ experiment considered here. As water began to infiltrate into the buffer, a rate of adsorption would dictate the amount and movement of water being adsorbed into the micropores. As a first approximation, the rate of adsorption is assumed constant for this analysis.

In the Buffer/Container Experiment, the experimental results showed that the temperature was in excess of 60°C (see Section 6.3.1, Figure 6.5 – 6.6). The high temperature in the engineered barrier was initially believed to have an effect on the adsorbed water in the clay layers, to the extent of destabilising or even de-bonding the hydrate contacts. From a thermodynamic point of view, an increase in temperature would result in an increase in the thermal vibration, leading to instability in the adsorbed layer. However, using Gouy-Chapman’s equation, Mitchell (1976) was able to demonstrate that temperature between 0°C to 60°C has little effect on the adsorbed layer. Pusch (1983) also reported that the temperature gradient and absolute temperature did not appear to have a controlling influence on the rate and distribution of water uptake. Later, Pusch et al., (1990) revealed that clay with a saturated bulk density of about 2 g/cm³ has dominant 1-hydrate interlamellar contacts. Such contacts were found to be insensitive to temperature below 100-120°C or pressure below 100 MPa. Additionally, they also concluded that the hydraulic conductivity for clay was controlled predominantly by viscosity. As the sand-bentonite material used in the Buffer/Container Experiment had a bulk density value in excess of 2 g/cm³, it is therefore reasonable to assume that the adsorbed water layer in the buffer would be largely unaffected by any temperature increase experienced in the experiment performed.

Figure 6.34 illustrates an idealised representation of a proposed conceptual model for the transient behaviour of adsorbed and free water within a clay-water system. The
following equations express the mathematical form of the assumed transient wetting/drying behaviour in clays.

The degree of saturation for a soil system comprises the adsorbed and free water components. This can be expressed as;

\[ S_{r_T} = S_{r_f} + S_{r_{ab}} \]  

(6.2)

where \( S_{r_T} \) represents the degree of saturation for the soil system, \( S_{r_f} \) represents the degree of saturation for free water, and \( S_{r_{ab}} \) represents the degree of saturation for adsorbed water.

In addition, the adsorption or de-sorption of water from a clay-water system can be represented by the following expression;

\[ S_{r_{ab}(j)} = S_{r_{ab}(i)} + \Delta S_{r_{ab}} \]  

(6.3)

where the subscripts \( j \) and \( i \) represent the final and initial values respectively, \( \Delta S_{r_{ab}} \) represents a change in the degree of saturation for adsorbed water.

As described earlier, a linear form of rate of adsorption was assumed and used to dictate the rate at which water is adsorbed into the clay intra-layers. This can be mathematically described as;

\[ r = \frac{w_{ab}(j) - w_{ab}(i)}{w_{\text{max}}} \times \frac{1}{T} \]  

(6.4)

where \( r \) represents the rate of adsorption, \( w_{ab} \) represents the percentage of total water that has been adsorbed, \( w_{\text{max}} \) represents the maximum percentage of total water which can be adsorbed (during steady state), \( T \) represents the total time taken. The graphical representation of Equation 6.4 is illustrated in Figure 6.35.

The term \( w_{ab} \) can also be expressed mathematically as;

\[ w_{ab} = \frac{S_{r_{ab}}}{S_{r_T}} \]  

(6.5)

Substituting Equation 6.5 into Equation 6.4 gives;
Rearranging Equation 6.6 yields;

$$\Delta S_{ra\,h} = r \times w_{max} \times T \times S_{r,T}$$

(6.7)

where $\Delta S_{ra\,h}$ represents the change in the degree of saturation for adsorbed water. Hence $S_{ra\,h}$ for the next iteration in a numerical model can be represented as;

$$S_{ra\,h(i+1)} = S_{ra\,h(i-1)} + \Delta S_{ra\,h}$$

(6.8)

Where the subscript $(i-1)$ represents the previous timestep and $(i+1)$ represents the next iteration.

$$w_f = 1 - w_{ab}$$

(6.9)

Finally, the percentage of total water considered free, $w_f$ (described in Equation 6.9) is calculated and applied to the swelling hydraulic conductivity equation (shown in Equation 6.1). The effective hydraulic conductivity can then be evaluated.

In the proposed conceptual model, when hydration occurs, the new arrival of water would be considered as free water. As dictated by the rate of adsorption, the free water would then be progressively adsorbed into the micropores until $w_{max}$ for the clay material is reached. It is also postulated that no further adsorption would take place unless this equilibrium state is disturbed by further addition of water. In the case of drying, free water would be removed first, followed by adsorbed water which is strongly held by electrostatic forces. During drying, when $w_{ab}$ exceeds $w_{max}$, it is assumed that water in the adsorbed layer would begin to de-sorp back into free water state. This continues until the steady state is reached.

The transient micro-macro model described above has been incorporated into the numerical model where a constant rate of adsorption and desorption rate were assumed. As the sand-bentonite buffer material had been placed in the emplacement borehole for more than 170 days before the heating phase was initiated, a maximum
permissible ratio of adsorbed water to total water of 94% was assumed at the start of
the simulation. Earlier in Section 6.7, it has been demonstrated that instead of
completely choking the flow of water as buffer approaches saturation, retarding the
movement of water yielded better correlation with experimental results. Hence, it was
decided to adopt $M_t$ as 1.0 in Equation 6.1 for this analysis. To evaluate the influence
of including a micro-macro transient modelling of the clay-water system, four sets of
numerical analyses which implement varying adsorption rates of $1.0 \times 10^{-5} \text{ s}^{-1}$, $5.0 \times
10^{-8} \text{ s}^{-1}$, $1.0 \times 10^{-8} \text{ s}^{-1}$ and $1.0 \times 10^{-9} \text{ s}^{-1}$ were carried out. The following sections
describe the numerical results obtained and how they compare against the
experimental results.

6.8.2 Comparison between Numerical results and Experimental results

The numerical pore water pressure results in the buffer are displayed in Figure 6.36
and 6.37. Compared with the experimental contour plots, correlations with varying
likeness were obtained for the four simulations which used different adsorption rate.
The numerical simulation that adopted an adsorption rate, $r$, of $1.0 \times 10^{-5}$ was taken
as a benchmark case where the adsorption rate was sufficiently high that even when
drying or wetting had occurred, the steady state can be achieved almost
instantaneously. The numerical results for this case should be similar to those
obtained in Section 6.7 where the adsorbed water was fixed at 94% throughout the
heating phase of the experiment. Observing both sets of results, there was little
difference between them. Hence, some confidence has been gained that in the
implementation of the modified numerical model incorporating the transient
behaviour for the water-clay system.

Figure 6.36 and 6.37 illustrate the contour plots for suction in the buffer at day 60,
day 150 and day 525. The bottom of the buffer gets wetter as the rate of adsorption
decreases. The pore water pressure contour plots in the near field rock were plotted
for day 30, day 150 and day 400 respectively in Figure 6.38 and 6.39. The variation
of adsorption produced significant changes in the moisture field in the rock. At the
beginning, the moisture field in the near field rock for the different adsorption rates
were similar. However, as the simulation progressed, a decrease in the adsorption rate
was met with a lesser pressure build up in the near field rock. As the adsorption rate
decreases, not all water is adsorbed immediately. Instead, the buffer would allow more free water to flow which increases the material’s permeability. Implicitly, as the buffer near the rock approaches saturation, the retardation effect would be slowed.

Observing the graph shown previously in Figure 6.29, when the buffer material approaches saturation, an increase in the adsorbed water content within the clay-water system would give a lower hydraulic conductivity. Hence, even as the buffer-granite interface is fully saturated, the availability of free water which is responsible for the bulk flow of moisture meant that movement of fluid is still possible. This is evident from the contour plots shown in Figure 6.38 and 6.39 where the pressure was building up at a slower rate. However, when the adsorption rate is assumed as high, the pressure in the near field rock was much higher. It is postulated that as free water arrives, water could be easily adsorbed into the micropores, causing swelling and inhibiting flow.

As discussed earlier, pore water pressure at the bottom of the buffer was much higher when using a high adsorption rate. This was thought to be due to the swelling at the interface. The pressure contour plots for the surrounding rock suggests that the rock would remain unsaturated near the top of the backfill and buffer materials. The rock is in contact with the exposed cavern, resulting in a slower recovery of the pre-construction water table.

The transient pore water pressure profiles in the rock for the investigation on the micro-macro structure influence on swelling are plotted in Figure 6.40, 6.41, 6.42 and 6.43 respectively. These simulated results provide further hints at the influence of the micro-macro factor in swelling clay. Similar to what was discussed earlier, as the swelling effect becomes effective at an early stage, the micropores become saturated and retard the moisture flow. Also, the rate of pressure build up at the interface is likely to be affected by the significance of swelling effects.

During this investigation on the transient nature of moisture movement between the micropores and macropores, the rate of adsorption and desorption effects the predictions for the Buffer/Container Experiment. The manner in which free water converts into adsorbed water and vice-versa is seen as an important feature in describing this experiment set up. The physical preparation of the clay buffer
material, the external pressure gradient imposed at the buffer interface as well as the
duration of an experiment could affect the rates of moisture transfers. The author is
aware that the present constant rates assumed for this Buffer/Container Experiment
are simplistic. However, it is strongly believed that the numerical model has
demonstrated its potential to simulate the moisture field behaviour in the
Buffer/Container Experiment.

Having observed the effects made by considering the roles of micro-macro structure
and its effect on swelling in the simulations, comparisons were made against the
experimental results to determine a suitable rate of adsorption. Based on the
correlations obtained, it was found that an adsorption rate of $1.0 \times 10^{-9}$ s$^{-1}$ gave the
closest prediction. The higher adsorption rates ($1.0 \times 10^{-8}$ s$^{-1}$ and $5.0 \times 10^{-8}$ s$^{-1}$) were
found to over-predict the rate of pressure build up in the rocks and the swelling effect
simulated was overestimated. Hence, both values were considered inaccurate and
have been eliminated. As such, the adsorption rate of $1.0 \times 10^{-9}$ s$^{-1}$ has been adopted
for subsequent analyses.

Although the experimental suction contour plot in the buffer at day 525 had much
less drying above and below the heater when compared with the numerical result for
this rate of adsorption, the end-of-test moisture content results displayed in Figure
6.11 indicate the buffer above and below the heater to be much drier. As mentioned
previously, Graham et al., (1997) believed that the end-of-test results produced better
representation of the Buffer/Container Experiment at its final stage than those
obtained from the thermal needles and psychrometers.

6.8.3 Conclusions

It has been demonstrated that a good overall correlation with the experimental results
can be achieved using the transient micro-macro hydraulic conductivity relationship.
The rate of water uptake and pore water pressure distribution in the engineered buffer
material and the host rock were both close to the actual experiment results. The
transient micro-macro relationship seems capable of accounting for the gradual
pressure build up recorded along the buffer-granite interface in the actual experiment.
In response to the improvements achieved for the inclusion of a transient micro-
macro influence on swelling, the same approach was extended to the
thermo/hydro/mechanical analysis.

6.9 Thermo/Hydro/Mechanical Simulation of the Heating Period (Phase D) in the Buffer/Container Experiment

Following the investigations on the coupling process of the thermal and hydraulic fields and the influence of microstructures on the overall swelling phenomena, the deformation effect has been included in the numerical model. Several changes have been introduced for the numerical model. The following sections detail the prescribed conditions for the numerical model and the simulation results obtained from the analysis.

6.9.1 Modifications and Prescribed Conditions for the Simulation

The thermal and hydraulic parameters used in the analysis described in Section 6.8 were again used in the deformation analysis. Similar initial and boundary conditions as well as the time stepping scheme used in the earlier thermal hydraulic simulations were applied.

Studies have found that preventing deformation within the rock has negligible influence on the stress development in the buffer for AECL’s Isothermal Experiment (Mitchell, 2002). Hence, a similar approach has been adopted here. Another advantage gained from adopting this approach is it significantly reduces the computational effort required for a full scale thermo/hydro/mechanical simulation. The top of the backfill was restrained from deforming in the vertical direction as the concrete cap and restraints rest on top of the engineered materials. A uniform initial isotropic stress of 200 kPa was assumed for the buffer, based on the experimental values shown in Figure 6.12. The sand was also assumed to be restrained completely. It is thought that the sand was well compacted around the heater by the buffer material and was not expected to deform.

The inclusion of deformation on the overall buffer material’s response is likely to affect the moisture movement. When expansion or contraction occurs within the buffer material, the overall void ratio would be affected. As a result, the amount of moisture required for the material to reach full saturation would be different. To
account for the deformation effects on the buffer material, a deformation parameter needs to be incorporated in the existing micro-macro swelling hydraulic conductivity relationship. Following the approach presented by Mitchell (2002) who utilised the void ratio parameter to elucidate the deformation effects, the modified hydraulic conductivity relationship is presented as follows:

\[
k_{\text{swell}} = k \times \left( \frac{e_i}{e} \right)^\alpha \left[ S_a + w_f S_i \left( \exp \left( (1 - w_f)M/S_i \right) \right) \right]
\]

(6.10)

where \(e_i\) is the initial void ratio in the clay, and \(\alpha\) is a constant which accommodates the degree to which the soil is restrained. Mitchell (2002) suggested a value of 1.0 for \(\alpha\) as the buffer was restrained by the surrounding rock and the restraining cap. This value has been adopted for this simulation. \(w_f\) follows the wetting and drying relationship shown in Figure 6.34.

Investigations on the effects of microstructure on the Buffer/Container Experiment have been described in Section 6.8. As described earlier, an adsorption rate of \(1.0 \times 10^{-9} \text{ s}^{-1}\) gave the closest fit to the actual experimental results, and was subsequently adopted in the analysis.

The following sections describe the simulation results obtained and the deformation effect on the numerical analysis.

6.9.2 Moisture and temperature results in the buffer and the rock

The thermal response obtained from the deformation analysis showed little difference when compared with the thermal hydraulic simulation. The results essentially matched those shown previously in Figure 6.17 and 6.18, and are not repeated here.

Figure 6.44a presents the pore water pressure contour plots in the buffer. When compared with the experimental contour plots obtained using the thermal needles and psychrometers, a good overall correlation was obtained. In the deformation analysis, there was less drying above and below the heater. This is much closer to the recorded experimental results. Figure 6.44b shows the pore water pressure contour plots in the near field rock. Compared with the plots obtained from the thermal hydraulic analysis, the pressure build up in the buffer rock interface was slower in the
deformation analysis. Figure 6.45 presents the transient pore water pressure profiles in the rock. Again, good correlations were measured against the readings from the hydraulic packers and piezometers.

The inclusion of the deformation effects have shown some differences in the moisture profile simulation results. As the buffer heats up, void ratio in the swelling clay begins to increase. Consequently, more moisture would need to be adsorbed into the buffer before it reaches a saturated state, thus delaying the onset of a pressure build up. The choking effect is also less severe in the deformation analysis. As such, water is able to flow into the engineered materials with less difficulty.

6.9.3 Stress-Strain Response in the Buffer Material

In this section, the horizontal and vertical stresses developed during the heating phase, as well as the predicted horizontal and vertical displacements are discussed and presented here.

6.9.3.1 Horizontal and Vertical Stress Profiles

Figure 6.46 and 6.47 present the horizontal stress profiles at mid-height of the heater and at vertical sections for the Buffer/Container Experiment. Observing the stress profile at mid-height of the heater, the horizontal stress profile across the length of the buffer increases at the same rate. As described earlier, there are two main causes of moisture movement. They have been identified as the infiltration of water at the buffer-granite interface and the vapour transfer from the heated region. The build-up of moisture in the buffer material results in increasing swelling pressures and accounts for the horizontal stress increase at mid-height of the heater.

Inspecting the horizontal pressure plots at vertical sections, the stress increases with increasing radial distance from the heater. It is postulated that the swelling at the buffer granite interface and the thermal shrinkage in the buffer near the heater resulted in the higher swelling pressure near the rock. The maximum simulated horizontal stress was initially positioned near the mid-height level of the heater. However, at later stages, the highest horizontal stress recorded was near the bottom of the buffer material. It is postulated that at the beginning, the thinner buffer layer at
the mid-height level experienced a higher temperature increase compared to buffer materials found elsewhere. This resulted in a sharp rise in the stress profile at the mid-height of the heater. However, as the simulation progressed, moisture was beginning to infiltrate into the bottom end of the buffer material. The larger volume of the buffer material at the bottom end would then produce a higher swelling pressure than the buffer materials at the mid-height level of the heater.

The vertical stress profiles at mid-height of the heater and at other vertical sections have been shown in Figure 6.48 and 6.49. Similar trends to those obtained for the horizontal stresses plots were obtained. Compared with the experiment results for total pressure (see Figure 6.12), a good qualitative match was observed. However, the simulated stresses were much higher than the actual experimental results. Several factors were thought to have contributed to these discrepancies. It was postulated that the assumption made on the incompressibility of sand may not have been entirely accurate. The sand may have been able to relieve part of the pressure build up during the course of the experiment. Also, construction of the borehole may have formed small cracks on the granite walls (an excavation damaged zone), which could allow buffer material being able to expand into the fissured rock when swelling occurs. This would relieve some of the stress build-up. Although the top of the buffer was held by concrete cap and restraints, it was suggested that seasonal temperature variation could cause the restraints to swell and shrink, thus providing some form of relieving effects.

6.9.3.2 Void Ratio

Figure 6.50a presents a profile of void ratio along mid-height of the heater. Observing the simulated results, void ratio in the buffer material near the heater can be seen gradually decreasing whilst the buffer material near the granite rock progressively increasing. It is postulated that the thermal and hydraulic responses were both responsible for the deformation changes experienced in the Buffer/Container Experiment. As the heater is activated, temperature gradients result in vapour flowing to cooler regions. The loss of moisture causes shrinkage in the buffer material near the heater. It is also suggested that the thermal expansion in the buffer materials near the rock has resulted in void ratio increases. The moisture flow
from the rock into the buffer system is also thought to affect the void changes in the buffer near the rock. The hydraulic gradient between the unsaturated sand-bentonite buffer and the rock results in moisture infiltrating into the buffer-granite interface. As the micropores becomes saturated, swelling occurs and soil begins to expand. The deformation analysis also suggests that the deformation experienced in the buffer along the mid-height of the heater had stabilised towards the end of the simulation.

In Figure 6.50b, the void ratio at a radius 0.39 m away from the centre of the borehole is also presented. It can be seen that the void ratio in the buffer next to the heater is experiencing significant change compared to the buffer material above and below the heater. As mentioned above, the drying induced shrinkage in the buffer material next to the heater is thought to be responsible for the reduction in void ratio. It is also postulated that as the sand-bentonite buffer above and below the heater has a much larger volume, deformations in these regions are less significant.

6.9.3.3 Horizontal and Vertical Displacements

Figure 6.51 and Figure 6.52 show the horizontal displacement at mid-height of the heater and vertical sections at varying radius lengths for the Buffer/Container Experiment. Observing the displacement profile in Figure 6.51, the buffer material is displacing towards the heater. As expected, this correlates well with the trends obtained from the simulated stress and void ratio profiles. Although no displacement measurements were made in the actual experiment, the simulated movements for the buffer material was qualitatively sound when compared with the experimental pressure plots.

The vertical displacement profiles are shown in Figure 6.53 and 6.54. The vertical displacement profile along the mid-height of the heater suggests that the buffer material was heaving upwards. It is postulated that resaturation in the buffer at the bottom end of the borehole meant that swelling would occur, resulting in an overall upward movement. Besides that, the backfill material at the top of the buffer is less dense compared to the buffer material, and compaction of this region would help relieve the pressure build up.
6.9.4 Conclusions

The thermo/hydro/mechanical simulation has managed to produce good overall correlation when compared with the experimental results. When the heater is activated, temperature increase is observed near the heater and water vapour escapes to cooler regions. As a result, drying shrinkage occurs in the buffer materials near the heater. In addition, the hydraulic gradient between the buffer material and granite rock encourages moisture to infiltrate into the buffer-rock interface. During resaturation, micropores in the buffer material adjacent to the rock would become saturated and subsequently retard moisture movement. This would also create swelling in the buffer near the granite rock. As described in the transient micro macro structure swelling mechanism, not all moisture is adsorbed immediately in the buffer material. Consequently, the pressure build up in the rock is gradual. Observing the stress development in the engineered buffer, the stress increases throughout the heating experiment. At the beginning, the maximum stress is recorded at the mid-height of the heater. However, towards to end of the heating experiment, this had shifted to the bottom of the buffer. It is postulated that as the large volume of the sand-bentonite material below the heater becomes saturated towards the end of the experiment, the swelling that occurs produces a large stress build up.

The inclusion of deformation effects in the analysis has certainly provided a better understanding on the thermal, hydraulic and mechanical response in the Buffer/Container Experiment. However, the numerical investigations carried out thus far on the performance of this in situ experiment have revealed several key parameters used in the simulation which are thought to affect the system's performance. The following section sets out to investigate these identified parameters.

6.10 Sensitivity analysis on some critical aspect for the simulation of the Buffer/Container Experiment

The engineered buffer material acts as one of the protective layers and serves to retard the movement of radionuclide in the high-level nuclear waste canisters towards the surrounding environment. One of the many key research areas is to establish a
thorough understanding on the soil interaction between the host rock and the engineered barrier.

Moisture flow in the buffer material affects the heat energy movement near the heater via variations in thermal conductivities and the resaturation process. Heat and moisture transport via vapour diffusion is also thought to be a critical consideration as it affects the evaporation and condensation process in the buffer materials. It has been demonstrated from the numerical analysis that the numerical model (which applies the transient exchanges between free and adsorbed water conceptual model) is able to provide good overall correlation. Hence, the numerical model was used to carry out further parametric studies, concentrating on the variation of the saturated hydraulic conductivity in the buffer material and a study on the effects of soil’s microstructure on vapour flow. The results are presented in the following sections.

6.10.1 Sensitivity analysis on the variation of the saturated hydraulic conductivity for Buffer Material in the Buffer/Container Experiment

6.10.1.1 Introduction

Studies have shown that the saturated hydraulic conductivity for bentonite clay (the preferred material for the buffer system) ranges from $10^{-10}$ m/s to $10^{-14}$ m/s. As such, sensitivity analyses which are subsequently compared with the simulation work presented earlier in Section 6.8 are presented in this section. The sand-bentonite’s saturated flow rate was varied over three orders of magnitude at $10^{-10}$ m/s, $10^{-11}$ m/s and $10^{-12}$ m/s (benchmark case). All other aspects of the simulation have been held constant.

For the sensitivity analyses, all material parameters, initial and boundary conditions are as described in Section 6.8 except for the hydraulic conductivity.

6.10.1.2 Numerical Simulations and Discussions

The simulated pore water pressure contour plots in the buffer at day 30, day 150 and day 525 using different saturated hydraulic conductivity are shown in Figure 6.55. In Figure 6.56, the transient contour plots for pore water pressure in the near field rock are displayed. Observing Figure 6.55, the simulated suction profile in the buffer
(using saturated flow rate of \(10^{10}\) m/s) displayed a slow and gradual resaturation. The drying effect observed near the heater is also less significant. However, as the applied saturated conductivity decreases, the suction difference between the buffer material adjacent to the heater and the buffer material near the rock increases significantly. Observing Figure 6.56, it can be seen that as the saturated rate of flow is reduced, pressure build up in the near field rock becomes significant. It is postulated that when the buffer’s saturated hydraulic conductivity is high, water can flow easily into the unsaturated buffer material. Although the micropores are saturated and swelling has occurred at the buffer-rock interface, it is not thought to be sufficient to retard the moisture movement into the buffer material. Conversely, when the saturated rate of flow is low, water entering via the buffer-granite interface will be adsorbed onto the clay interlamellar layer. As the buffer material reaches saturation, water movement is retarded and the delayed arrival of water into the buffer near the heater causes it to become even drier (due to the heating). In addition, the ‘choking’ of flow is also thought to allow the pore water pressure in the near field rock to recharge.

Figure 6.57 presents the degree of saturation profiles obtained from the simulations. Figure 6.58 shows the degree of saturation changes with time in the buffer and the near field rock. It can be seen that similar trends such as those described above are observed. Observing 6.57, when the applied saturated hydraulic conductivity is \(10^{10}\) m/s, no significant drying effect can be detected. It appears that moisture has little difficulty resaturating the buffer material. However, as the permeability is reduced, the drying becomes more pronounced near the heater and the buffer-granite interface was fully resaturated by day 100. The swelling at the buffer-granite interface is preventing moisture from flowing towards the dry buffer region.

6.10.1.3 Conclusions

The parametric study on the saturated hydraulic conductivity for the clay-based material used in the Buffer/Container Experiment’s simulation has a huge impact on the resaturation behaviour and performance of the design as a whole. When a bentonite-clay with low hydraulic conductivity is applied, swelling is likely to occur early in the experiment, accompanied by a significant drying effect near the heater. Despite a large difference in suction between the buffer material near the heater and
the buffer material adjacent to the rock, the suction imbalance continues as the swelling retards moisture from flowing. However, when using a buffer material with high hydraulic conductivity, the drying and swelling effects become insignificant as moisture is able to flow rapidly and resaturate the engineered system.

6.10.2 Sensitivity Analysis on Vapour Diffusion in the Buffer material

6.10.2.1 Introduction

The cycle of evaporation and condensation has huge implication on the resaturation process in a heating experiment for an engineered barrier. In the numerical model used to simulate the Buffer/Container Experiment, the Philip and de Vries (1957) mechanistic approach to moisture flow was applied. However, this approach was developed from experimental works on cohesionless materials. In the Buffer/Container Experiment performed by AECL, the sand-bentonite buffer material is a cohesive material with high swelling potential. It is thought that the vapour flow transfer in a cohesionless material is quite different from a cohesive material with intricate micro-macro structure. Cleall et al. (2002) found that the calibrations of the temperature effect factor \( D_{TV} \) and the suction effect factor \( D_{MV} \) were able to account for the vapour velocity in bentonites. The Philip and de Vries vapour velocity equation has been presented in Chapter 3 and only a general form of the equation is presented here:

\[
v_v = D_{TV} \left( h \frac{\partial \rho_0}{\partial T} + \rho_0 \frac{\partial h}{\partial T} \right) \nabla T - D_{MV} \left( \rho_0 \frac{\partial h}{\partial s} \right) \nabla s \quad (6.11)
\]

A sensitivity analysis was performed where the \( D_{MV} \) term was held constant and the \( D_{TV} \) term which determines the level of influence temperature has on the vapour velocity were varied at 0.2, 0.6 and 1.0 respectively. The rest of the parameters and boundary conditions were left unchanged. The results are shown in the next section.

6.10.2.2 Numerical simulation and discussions

The pore water pressure contour plots in the buffer material and the near field rock are presented in Figure 6.59 and 6.60. As the heater was switched on, the drying effect experienced in the buffer near the heater became less significant as the
influence temperature has on the vapour flow was reduced. Observing the contour plots in the rock, there was little variation in the pore water pressure distribution for the near field rock. However it can be seen that at day 150, the pressure build up was much faster as the vapour flow factor was increased.

The pore water pressure profiles along the mid-height of the heater are presented in Figure 6.61. It can be seen that as the coefficient of vapour diffusion ($D_{TV}$) decreases, the pressure build up at the buffer-granite interface becomes less significant. The reduction of the temperature effect on vapour velocity resulted in the air void within the micro-macro model becoming saturated at an earlier stage. As such, evaporation becomes more difficult and the lack in vapour transfer meant that little condensation at the cooler buffer region would occur. Towards the end of the experiment, the pressure build up in the buffer near rock and the near field rock were generally similar for all three simulations. It is postulated that although variation in the coefficient of vapour diffusion ($D_{TV}$) may have affected the evaporation-condensation cycle in the buffer material, moisture would eventually infiltrate into the buffer-rock interface, causing swelling to occur.

6.10.2.3 Conclusions

It has been demonstrated that the vapour diffusion terms in the Philip and de Vries approach used in the numerical formulation requires careful consideration. During heating, moisture movement would occur and some of the micropores may become saturated. Swelling in the micropores would reduce the existing macropore voids, thus restricting the available flow paths for vapour transfer. In the parametric studies on vapour transfer in clayey soils, the change in vapour velocity affects the evaporation process near the heater and consequently the resaturation effort.

6.11 Conclusions

The numerical code COMPASS was used to perform a series of simulations on the thermal, hydraulic and mechanical behaviour of the AECL’s Buffer/Container Experiment. A thermal hydraulic analysis was initially performed using the original hydraulic conductivity relationship for the buffer as described in Chapter 5. An
excellent correlation was achieved between the experimental transient temperature results and the numerical transient temperature results. However, the pore water pressures in the buffer and the rock did not correlate as well. It was thought that the swelling phenomena had not been properly accounted for.

An exponential hydraulic conductivity relationship proposed by Mitchell (2002) was included to account for the buffer material's swelling behaviour. The correlation between the simulated and experimentally obtained pore water pressure results showed improvements. However, the pore water pressure build up in the rock was over-estimated in the simulation. It was believed that the movement of water should not be completely restricted when the buffer is saturated.

An investigation was then carried out on the proposed relationship representing the swelling phenomena. The choking mechanism in the buffer-rock interface was relaxed to allow moisture to flow through albeit at a reduced rate. This approach provided an improved correlation when compared with the pore water pressure experimental results. However, it was thought that the swelling phenomena had yet to be captured correctly.

A conceptual model representing transient free-adsorbed water transfer within a clay-water system was proposed for the numerical model where a constant adsorption and desorption rate were assumed for the analysis. An overall good correlation was achieved when comparing the simulated pore water pressure results with the actual pore water pressure experimental results. When the numerical model was extended to include the deformation effects, similar trends in the temperature and suction fields were observed in both the thermal hydraulic and thermo/hydro/mechanical analysis. Good qualitative comparisons were also measured when comparing the numerical and experimental results for stress/strain development.

Parametric studies have also been performed on the inherent permeability of clay-based buffer material and the effects of limiting vapour diffusion on the evaporation-condensation cycle. As the engineered buffer's saturated hydraulic conductivity increases, the drying effect becomes less pronounced and the pressure build up near the rock is less significant. This suggests that a high flow rate would negate any swelling occurring in the buffer-rock interface. On the effects of vapour diffusion in
the buffer material, microstructure in the clay could potentially restrict vapour movement and affect the resaturation effort in the emplaced system.

The ability to predict and simulate the thermal and hydraulic response, as well as the stress-strain behaviour in an underground repository is an important step towards the realisation of an active underground waste disposal unit. The proposed transient micro-macro structure swelling model is believed to be capable of describing the swelling effect in the Buffer/Container Experiment and the buffer-rock interactions.

6.12 References

AECL, (2002) Personal communication via E-mail.


<table>
<thead>
<tr>
<th>Label</th>
<th>Period</th>
<th>duration (days)</th>
<th>Type of work</th>
</tr>
</thead>
</table>
| A     | 6\textsuperscript{th} Aug 1990 – 13\textsuperscript{th} May 1991 | 280 | • Drilling the emplacement borehole  
• Monitor the effect of the drilling on water pressures and fluxes |
| B     | 13\textsuperscript{th} May 1991 – 13\textsuperscript{th} Sep 1991 | 30 | • Installation of buffer, backfill heater, and the accompanying instrumentation in the borehole |
| C     | 13\textsuperscript{th} Sep 1991 – 20\textsuperscript{th} Nov 1991 | 170 | • a dwell period during which temperatures, total pressures, and water pressures were stabilising towards values operative at the beginning of the heating experiment |
| D     | 20\textsuperscript{th} Nov 1991 – 5\textsuperscript{th} May 1994 | 897 | • heating period with power applied to the heater for a total of 897 days of continuous operation |
| E     | 5\textsuperscript{th} May 1994 – 13\textsuperscript{th} May 1994 | 9 | • decommissioning phase in which the buffer and the instrumentation were removed from the emplacement borehole |
| F     | 13\textsuperscript{th} May 1994 – 28\textsuperscript{th} Dec 1995 | 230 | • a follow-up period after the experiment during which water pressures and temperatures continued to be read in the host rock |

Table 6.1 Description of each phase for the Buffer/Container Experiment
### Table 6.2 Location of the piezometers in AECL’s Buffer/Container Experiment

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Radius (m) from the centre of the borehole</th>
<th>Elevation (m) relative to the centre of the heater</th>
<th>Registering negative pore water pressure</th>
</tr>
</thead>
<tbody>
<tr>
<td>1RH1</td>
<td>0.834</td>
<td>+1.577</td>
<td>Yes</td>
</tr>
<tr>
<td>1RH2</td>
<td>0.865</td>
<td>+0.014</td>
<td>Yes</td>
</tr>
<tr>
<td>1RH3</td>
<td>0.87</td>
<td>-0.92</td>
<td>Yes</td>
</tr>
<tr>
<td>1RH4</td>
<td>0.87</td>
<td>-1.82</td>
<td>Yes</td>
</tr>
<tr>
<td>1RP2M</td>
<td>1.06</td>
<td>+0.1</td>
<td>Yes</td>
</tr>
<tr>
<td>1RP3M</td>
<td>1.35</td>
<td>+0.1</td>
<td>Yes</td>
</tr>
<tr>
<td>1RP4M</td>
<td>1.71</td>
<td>+0.02</td>
<td>Yes</td>
</tr>
<tr>
<td>1RP5M</td>
<td>2.03</td>
<td>+0.03</td>
<td>Yes</td>
</tr>
<tr>
<td>1RP6M</td>
<td>2.42</td>
<td>+0.04</td>
<td>No</td>
</tr>
<tr>
<td>1RP7M</td>
<td>2.81</td>
<td>+0.05</td>
<td>No</td>
</tr>
</tbody>
</table>
Figure 6.1 Schematic layout of AECL’s concept for deep disposal of nuclear waste (after Graham et al., 1997)
Figure 6.2 Construction layout and dimensions of AECL's Buffer/Container Experiment (after Graham et al., 1997)
Figure 6.3  Section through the buffer showing: thermocouples (BT, FT), thermistors (BM), earth pressure cells (BR, FR), and thermal needles (BN), (after Graham et al., 1997)
Figure 6.4    Longitudinal section of Room 213 showing packer (HG) and thermistor (T) instrumentation in the rock (after Graham et al., 1997)
Figure 6.5 Experimental transient temperature profiles along mid-height of the heater
Figure 6.6 Experimental transient vertical temperature profiles through the emplacement borehole centre (N.B. in the heater region the experimental results represent the skin temperature of the heater)
Figure 6.7  Pore water pressures in the packer boreholes prior to placement of the buffer
Pore water pressures for the heating period - Experimental results for a 4 m x 8 m domain (after Graham et al., 1997)

Figure 6.8 Transient pore water pressures for the rock adjacent to the borehole
Figure 6.9 Pore water pressure profiles at varying depths in the granite rock.
Figure 6.10  Transient pore water pressure contours for the buffer (after Graham et al., 1997)
Figure 6.11  Comparison of the distributions of water contents from the thermal needles and psychrometers, and from the decommissioning water contents, (after Graham et al., 1997)
Figure 6.12  Transient total pressures in the buffer and the backfill (after Graham et al., 1997)
Figure 6.13 15m by 16m finite element mesh for the Buffer/Container Experiment (after Mitchell, 2002)
Figure 6.14  15 m x 30 m finite element mesh to find the draw down in pore water pressure following cavern construction and borehole drilling
Figure 6.15  Pore water pressure contour and profile along mid-height of buffer prior to start of heating period
Figure 6.16  Pore water pressures in the buffer following the ‘dwell’ period
Figure 6.17 Transient temperature results along mid-height of buffer during heating phase.
The experimental results in the heater region represent the skin temperature of the heater.

The numerical results are obtained in the sand annulus.

Figure 6.18  Transient temperature through the emplacement borehole centre
Figure 6.19 Transient pore water pressures in the rock during the heating period
Figure 6.20 Experimentally measured pore water pressures for packers HG8 and HG9
Figure 6.21 Transient pore water pressure profiles in the rock at various heights without swelling effects
Figure 6.22  Pore water pressure contours in the buffer, using the original hydraulic conductivity curve
Figure 6.23 Conceptual for the adsorbed and free water in clay model adopted for the buffer material in the Buffer/Container Experiment (Thomas et al., 2003)
Figure 6.24  Exponential Relationship to represent the swelling behaviour in the buffer
5879 nodes with 1832 8-noded quadrilateral elements

Figure 6.25  Refined Finite Element Mesh with Further Discretization in the buffer elements
Figure 6.26 Transient pore water pressures in the buffer, using an exponential correction for swelling in the numerical simulation.
Pore water pressures for the heating period
Numerical results including deformation and swelling
For a 4 m x 8 m area

Figure 6.27  Transient pore water pressures in the rock during the heating period, including swelling in the buffer
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Figure 6.30 Transient pore water pressures in the rock during the heating period, including swelling in the buffer for $M_f = 0.1$ and $M_f = 1$. 
Figure 6.31 Transient pore water pressures in the buffer, using an exponential correction with $M = 0.1$ and $M = 1.0$ for swelling in the numerical simulation.
Figure 6.32 Transient pore water pressure profiles in the rock at various heights using exponential relationship for $M = 0.1$
Figure 6.33  Transient pore water pressure profiles in the rock at various heights using exponential relationship for $M = 1.0$
Wetting Phase

Air

$w_f$

$w_{ab}$

SOLID

initial state

Pore air volume reducing

$w_f$ (increase)

$w_{ab}$ (no change)

intermediate

$w_f$ (decrease)

$w_{ab}$ (increase)

final state

Drying Phase

free water decrease

$w_f$

$w_{ab}$

SOLID

initial state

$w_f$ (increase)

$w_{ab}$ (no change)

intermediate

$w_f$ (decrease)

$w_{ab}$ (increase)

final state

When $w_{max}$ is exceeded during drying, free water recovery is initiated.

Adsorbed water increases after time, $T$

Free water increases until $w_{ab} = w_{max}$

Figure 6.34 An idealised representation of the conceptual model for transient behaviour of adsorbed/free water in clay
When $w_{\text{max}}$ is achieved, the term $w_w/w_{\text{max}}$ returns to 1.0.

Figure 6.35  Linear form of relationship adopted for the rate of adsorption.
Figure 6.36 Transient pore water pressures in the buffer using adsorption rate of $1.0 \times 10^{-5} \text{ s}^{-1}$ (top row) and $5.0 \times 10^{-8} \text{ s}^{-1}$ (bottom row)
Figure 6.37 Transient pore water pressures in the buffer using adsorption rate of $1.0 \times 10^8$ s$^{-1}$ (top row) and $1.0 \times 10^9$ s$^{-1}$ (bottom row).
Figure 6.38  Transient pore water pressures in the rock during the heating period, including transient micro-macro effect with adsorption rate of $1 \times 10^{-5}$ (top row) and $5 \times 10^{-8}$ (bottom row)
Figure 6.39  Transient pore water pressures in the rock during the heating period, including transient micro-macro effect with adsorption rate of $1 \times 10^{-8}$ (top row) and $1 \times 10^{-9}$ (bottom row).
Figure 6.40  Transient pore water pressure profiles in the rock at various heights using adsorption rate of $1.0 \times 10^{-5} \text{ s}^{-1}$
Figure 6.41 Transient pore water pressure profiles in the rock at various heights using adsorption rate of $5.0 \times 10^{-8} \text{ s}^{-1}$
Figure 6.42 Transient pore water pressure profiles in the rock at various heights using adsorption rate of $1.0 \times 10^{-8}$ s$^{-1}$
Figure 6.43 Transient pore water pressure profiles in the rock at various heights using adsorption rate of $1.0 \times 10^{-9}$ s$^{-1}$
Figure 6.44  Transient pore water pressures in the (a) buffer & (b) near field rock during the heating period, including deformation and swelling in the buffer.
Figure 6.45 Transient pore water pressure profiles in the rock at various heights including deformation effects and using micro-macro swelling hydraulic conductivity relationship.
Horizontal stress at mid-height of heater

Horizontal stress at a vertical section 0.03 m from the centre of the heater

Figure 6.46  Horizontal stress in the buffer, at the mid-height of the heater, and for vertical section at a radius of 0.03 m from the centre of the heater
Horizontal stress at a vertical section 0.39m away from centre of the heater

Horizontal stress 0.59m away from centre

Horizontal stress at a vertical section 0.59m away from the centre of the heater

Figure 6.47 Horizontal stress in the buffer for a vertical section at a radius of 0.39 m and 0.59 m from the centre of the heater
Vertical stress along mid-height of heater

Vertical stress at a vertical section 0.03 m away from centre of the heater

Figure 6.48  Vertical stress in the buffer for a vertical section along mid-height of heater, and at a radius of 0.03 m from the centre of the heater
Vertical stress at a vertical section 0.39 m away from centre of the heater

Vertical stress at a vertical section 0.59 m away from the centre of the heater

Figure 6.49  Vertical stress profile at a radius 0.39 m and 0.59 m away from centre of the heater
Figure 6.50 Void ratio profile along mid-height of the heater and at a radius 0.39m away from the centre of the heater
Horizontal displacement at a radius 0.03 m away from centre of heater

Figure 6.51 Horizontal displacement along mid-height of heater and at a radius 0.03 m away from centre of heater
Horizontal displacement at a radius 0.39 m away from centre of heater

Horizontal displacement at a radius 0.59 m away from centre of heater

Figure 6.52  Horizontal displacements at a radius 0.39 m and 0.59 m away from centre of heater
Figure 6.53  Vertical displacements along mid-height of heater, and at a radius 0.03 m away from centre of the heater
Vertical displacement at a radius 0.39 m away from centre of heater

Vertical displacement at a radius 0.59 m away from centre of heater

Figure 6.54  Vertical displacements at a radius 0.39 m and 0.59 m away from centre of the heater
Figure 6.55 Transient contour plots in the buffer using various hydraulic conductivities.
Figure 6.56 Transient contour plots in the rock with different saturated hydraulic conductivity
Figure 6.57  Degree saturation profile for various saturated hydraulic conductivities along mid-height of heater
Figure 6.58 Transient changes in the degree saturation at various points along the mid-height of the heater for parametric studies on saturated hydraulic conductivity
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Figure 6.60  Transient pore water pressure contour plots in the rock with varying vapour flow factor (vff) in the buffer.
Figure 6.61 Transient pore water pressure profile along mid-height of buffer (-3.0 m from top of buffer) with varying vapour flow factor.
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7.1 Introduction

Atomic Energy of Canada Limited (AECL) has performed a number of large scale in situ experiments, namely the Buffer Container Experiment and Isothermal Experiment. However, these experiments were based on a vertical borehole configuration. Another design concept being considered is the horizontal canister deposition configuration which involves placing canisters in horizontal boreholes from an access tunnel. According to a report published by Japan Nuclear Cycle Development Institute (2000), vertical canister configuration such as the Buffer/Container Experiment allows for better operability as the emplacement of waste canisters and engineered buffer materials is made easier. However, they believed that adopting a horizontal emplacement concept reduces the total excavated volume and the amount of backfill materials required. The concept was also thought to be more economical as the area of underground space demanded for the facility can be reduced.

The geometry layout for the In Room Emplacement was proposed by AECL as a potential design concept employing a horizontal canister deposition configuration. In the proposed experiment, the room is symmetrical with two set of canisters positioned at mid-height of a tunnel. Each canister is 1200 mm in diameter, 3870 mm long and surrounded by densely compacted engineered buffer material. This chapter
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presents a systematic full scale thermo/hydro/mechanical simulation of the proposed In-room geometry setup. For the remainder of this Chapter, the proposed emplacement system is referred to as the In-room geometry. Critical material factors such as the hydraulic conductivity relationship, threshold pressure for the surrounding granite rocks and the influence of hydrostatic pressure have also been investigated and discussed herein.

Section 7.2 details the proposed design layout for the In-room geometry and the finite element mesh used throughout the simulation of the designed geometry setup. Section 7.3 puts forward an outline of the thermal response in the In-room geometry due to heating from high level waste. In Section 7.4, a hydraulic only analysis is presented where an isothermal condition was assumed for the whole domain. Section 7.5 discusses a coupled thermal hydraulic simulation of the proposed geometry. Incorporating the transient micro-macro interaction as discussed in the previous chapter, a thermo/hydro/mechanical analysis of the considered design layout is presented in Section 7.6. Having predicted the In Room’s thermal, hydraulic and mechanical response, Section 7.7 investigates the effects of a saline condition on performance. In Section 7.8, a sensitivity study is carried out to investigate the influence of a threshold pressure in the granite rock on the emplaced system. Section 7.9 details an evaluation on the effect of variation of the hydrostatic pressure. Finally, Section 7.10 summarises the conclusions drawn from the simulations performed.

7.2  Design Layout for In-room geometry

As mentioned in Section 7.1, the In-room geometry was proposed by AECL (NWMO, 2004) as a potential horizontal canister deposition configuration. Figure 7.1 and Figure 7.2 respectively present a 3-D schematic overview of the proposed geometry and a typical cross-section of a single tunnel with both canisters next to each other at the mid-height of the tunnel. Figure 7.3 illustrates a plan view of the In-room geometry where the emplacement room length is 315 m, fitting 108 containers in the room with an end-to-end spacing of 1250 mm. Figure 7.4 presents a vertical cross-section of the room and details the positions and dimensions of the various design materials. In the proposed design, a cylindrical copper container is surrounded
by an inner buffer layer, followed by an outer buffer layer, a dense backfill layer and a light backfill layer. A layer of concrete of varying thickness is positioned at the bottom of the excavated room. Both excavation and tunnelling procedures are thought to affect the integrity of the rock formation adjacent to the exposed area. Hence, a 1.3 m thick layer of rock is regarded as an Excavation Damaged Zone (EDZ) to account for an expected increase in porosity and saturated flow rate.

The In-room geometry is a complex problem to simulate because of its complex and large scale geometrical configuration. Additionally, the coupled thermo/hydro/mechanical processes, as well as the interactions between adjacent materials further increase the numerical difficulties and computational demands. Hence a systematic modelling approach has been adopted to identify a suitable finite element mesh capable of describing the proposed configuration, as well as to assess the overall thermo/hydro/mechanical performance of the proposed geometry.

7.3 Thermal Simulation of the In-room geometry

The In-room geometry was simulated using the numerical model (COMPASS) described in Chapter 4. As shown earlier in Figure 7.3, the In-room Emplacement was proposed as consisting of a 315 m long and 7.14 m wide tunnel, which yields a high length to breadth ratio. Hence, it is not unreasonable to assume that the tunnel is semi-infinite. Observing the proposed geometry, the highest temperature and stress build-up are likely to occur at the centre of the room, along the line of symmetry of the geometry layout. The ends of the tunnels are also thought to be cooler than other parts of the proposed geometry as the surrounding granite rocks were able to absorb the generated heat readily. Another observation that can be made is that the excavated ends would be expected to yield negligible influence on the overall thermo/hydro/mechanical response in the emplaced system. In view of these observations, the tunnel ends' influence were ignored and the proposed geometry was simulated as a 2-D problem. As the proposed geometry is symmetrical about the vertical line midway between both canisters, the simulation considered just one half of the cross section as shown in Figure 7.4.
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Having established the geometry to be considered in a thermal simulation, a mesh was created. The mesh and time stepping schemes were checked for spatial and temporal convergence. The material parameters used in this numerical model have been described earlier in Chapter 5.

7.3.1 Thermal simulation to establish domain size and boundary conditions

Similar to the simulation for the Buffer/Container Experiment, a heat only analysis was performed to establish a reasonable domain size and its appropriate boundary conditions. Investigations found that a 100 m by 100 m mesh as illustrated in Figure 7.5 was suitable for the numerical analysis. As discussed above the In-room geometry has been simulated as a 2-D problem. The main objective for the thermal simulation is to initially assess the thermal response for the proposed configuration. The results obtained from this simulation are also used in Section 7.5 to compare against temperature profiles in a thermal hydraulic simulation.

7.3.2 Initial and boundary conditions

The In-room geometry is a proposed geometry for a horizontal canister deposition configuration. As such, the exact location and depth of placement are yet to be determined or finalised. To facilitate the simulation of this proposed geometry, assumptions have been made in the numerical model to predict the performance of the configuration when waste canisters are put in place. AECL (2002) has indicated that the initial temperature of the rock mass and emplaced system will be similar to the background temperature of AECL’s Underground Research Laboratory, measured at 286 K. This assumption has been included in the numerical model. The far field boundaries were fixed at their initial temperature of 286 K on surfaces CD, DB and AB. Numerical tests have confirmed that this fixity condition has a negligible effect on the near field temperature results. A zero flux boundary condition was applied onto the surface AC as shown in Figure 7.6 to represent the line of symmetry present in the cross section of the geometry. A heat flux that varies with time was applied onto the inner surface of the copper lining. A variable heat flux representing the gradual decay of a high level nuclear waste material, based on findings recorded in
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Tait et al., (2000) was used. The relationship which describes the heat output representative for each container is shown in Table 7.3 and Figure 7.7.

The initial time-step for this analysis was set at 1 second, and allowed to increase to a maximum time step of 2 years via the algorithm described in Section 4.4. The analysis was performed for a period of 1000 years. The material parameters used in the numerical model have been described in Chapter 5. Figure 7.6 provides a schematic overview of the initial and boundary conditions applied in the simulation. The following section describes the numerical results obtained.

7.3.3 Numerical Results

Results from the thermal simulation are shown in figures 7.8 - 7.14. Each individual contour plot is representative of the emplaced system; measuring 4.50 m by 5.80 m. Contour plots of similar dimensions will also be used in later sections.

Figure 7.8 presents the numerically simulated temperature contour plots at various times. It can be seen that on installation of the canister in the room, the temperature begins to rise, with a peak temperature observed at the surface of the copper container after 10 years. After 40 years, the effect of thermal loading begins to decrease as indicated by a lowering in the temperature.

Figure 7.9 illustrates the temperature variation with time at the surface of the canister, and in the light backfill, the inner EDZ and the near field host rock. Figure 7.10 shows the temperature profile along the mid-line of canister. The mid-line of the canister is an imaginary horizontal line across the diameter of the canister and extends through the mesh. An illustration of this line is projected in Figure 7.11.

Observing Figure 7.9, temperatures peaked earliest at the canister surface, followed by other parts of the emplaced system. As the temperature at the surface of the canister peaked, heat energy was gradually dissipating towards cooler regions, thus delaying the onset of maximum temperature in the light backfill, inner EDZ and host rock. The temperature difference between the surface of the canister and the host rock also began to reduce as the simulation progressed. Changes in temperature gradient at the materials' interfaces can be observed in Figure 7.10. The change was
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due to the different thermal conductivity relationship employed for each emplaced material.

The maximum simulated peak temperature of 398 K requires further consideration. In the analysis performed, the heater power was set to a value equivalent to having a continuous canister installed longitudinally through the tunnel. As mentioned previously, the end-to-end spacing in the suggested layout was proposed at 1.25 m, with the container length proposed at 3.87 m. It was considered that the gap in between containers could be accounted for via a reduction in the simulated heater power. A scaling factor based on the ratio between 'length of canister' and 'length of canister and spacing gap' was applied to lower the prescribed heat output used in the numerical model. This provides a more realistic heat flux for the thermal simulation. The 'reduced heat flux' relationship is also shown in Figure 7.7.

A second thermal analysis was then performed using this lower heat flux relationship. Figure 7.12 shows the simulated temperature contour plots at various periods. Figure 7.13 and 7.14 present the temperature variation with time and temperature profile at mid-line of the canister. Compared with the numerical results presented earlier for an unmodified heat flux, similar trends were obtained. However, the reduced-power numerical analysis produced a lower peak temperature of 376 K at the surface of canister.

The two sets of results could be considered to represent the upper and lower bound solution of the heat analysis. The upper bound (i.e. using unmodified heat flux) approach assumed the heater was continuous and gave a conservative (over-estimated) prediction of the thermal response for the In-room geometry. The lower bound (i.e. using a reduced heat flux) approach took into account the gap between canisters and provided a more realistic prediction of the thermal response. However it would tend to slightly under predict the temperature at the mid length of the canister, as it applied an average heat flux for the entire length of the tunnel. On balance, the author considered that the lower bound approach gave a more realistic representation of the emplaced system’s thermal response. In view of this, the lower bound approach was adopted for the thermal hydraulic and thermal/hydro/mechanical simulations of the In-room geometry.
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### 7.4 Hydraulic Simulation of the In-room Geometry

In this section an isothermal hydraulic numerical simulation of the In-room geometry is presented. The finite element mesh shown previously in Figure 7.5 was adopted for this simulation. Two sets of numerical results were obtained. The first set assumed no swelling effect for the bentonite-based buffer material used in the system. The second set incorporated the transient swelling exponential hydraulic conductivity relationship as presented in Section 6.8.

This analysis investigated the hydraulic response in the proposed In-room geometry as water began to enter from the surrounding saturated rock into the emplaced system. Comparisons are made between the hydraulic response for a model which ignored the swelling phenomena and a model which accounts for the swelling effect in bentonite-based materials.

#### 7.4.1 Initial and Boundary Conditions

The initial pore water pressures for the materials designed for the system have been determined from the materials’ water retention curve (presented in Chapter 5) based on the initial degree of saturation provided in Table 7.2 (AECL, 2002). The actual depth of the centre of tunnel has not yet been determined although AECL (2002) suggested the depth of placement to be between 500 m and 1000 m below ground level. In view of this, the In-room geometry was assumed to take place at 500 m below ground level.

Personal communication with AECL (2002) has also indicated that the pore water pressure in the surrounding rock can be assumed at hydrostatic pressure. The setting up of the proposed configuration would require tunnel excavation. The open tunnels would be left exposed for a period of time before operations and monitoring could begin. Such exposure at the tunnel surface would result in a draw-down effect. To represent this draw-down effect in the near field rock, the hydrostatic pressure in the far field rock (beyond 10 m) was assumed to reduce through the near field rock down to 0 Pa at the surface of the tunnel (AECL, 2002).
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The author has incorporated the assumptions described above to help define the initial and boundary conditions for pore water pressure within the rock. A zero flux boundary condition was assigned along the line of symmetry in the system. The time-stepping scheme used earlier in the heat analysis was again employed for the numerical analysis.

7.4.2 Numerical Results

Figure 7.15 – 7.17 present results from the analysis where the ‘standard’ hydraulic conductivity relationship has been used. Figure 7.15 presents the pore water pressure contour plots at various periods for the proposed geometry. It can be seen that the initial pore water pressure in each as-placed material was distinctly different from its neighbouring material. However, the pore water pressure contour gradient between adjacent materials began to reduce as the simulation progressed. Figure 7.15 also shows that water was infiltrating from the surrounding rocks into the unsaturated emplaced system.

Figure 7.16 and Figure 7.17 show the variation of degree of saturation with time at various materials in the system and along the mid-line of the canister. Both figures show that the re-saturation process was initiated from the onset of the hydraulic simulation, with complete re-saturation achieved after 110 years. The degree of saturation profiles in Figure 7.17 showed that steady state in the emplaced materials was reached after 3 years. As the emplaced system began to resaturate, a pore water pressure build up in the rocks was simulated.

The trends simulated in the analysis were as expected. The suction gradient between the saturated rock and the unsaturated emplaced materials encouraged moisture to flow towards the emplaced system, and eventually resaturating the In-room geometry.

However, the emplaced materials in the In-room geometry are restrained by the surrounding host rock. Earlier in Chapter 6, the Buffer/Container Experiment recorded a significant pore water pressure build up near the buffer-rock interface. The pressure build up was associated with swelling in the buffer material as moisture began infiltrating from the surrounding rock. The pressure build up was also believed to have affected the resaturation process. The simulation results obtained using the
transient swelling model showed good correlation with the measured experimental results. Hence, the transient micro-macro swelling model proposed in Section 6.8 has been extended for the inner and outer buffer in the In-room geometry. The clay contents and as-placed densities for both materials are high and would be expected to swell. Incorporating this hydraulic conductivity model, the isothermal hydraulic analysis was repeated and re-assessed. Similar for the Buffer/Container Experiment an adsorption rate of $1.0 \times 10^{-9}$ m/s was assumed for the In-room. A maximum permissible ratio of adsorbed water percentage to total water of 94% was assumed. The $M_f$ value (described in Equation 6.1) was again taken as 1.0.

Figure 7.18 and 7.19 show the contour plots and variation in degree of saturation with time at various positions along the midline of the heater canister using the transient swelling model. Compared with the earlier numerical results, the buffer material was observed to be re-saturating at a slower rate. The degree of saturation profiles for the inner and outer buffer were also different in the first 10 years for both sets of simulations. The higher degree of saturation gradient in the inner and outer buffer material indicates swelling at the materials' interface. As the resaturation process began, the degree of saturation in the outer layer of outer buffer began to increase. The introduction of the swelling relationship in the numerical model prevented water from seeping into the unsaturated buffer materials easily, and resulted in a slower resaturation in the inner layer of buffer.

In relation to the overall saturation profile, the inclusion of the swelling effect for the In-room geometry has affected the resaturation process. The retardation effect at the materials' interface has delayed the flow of moisture. It is thought that the inclusion of the swelling effect in the numerical model would present a more realistic representation of the emplaced system's hydraulic response.

### 7.4.3 Conclusion

The numerical simulation of the hydraulic response in an isothermal environment for the In-room geometry has indicated that complete resaturation would be achieved after 110 years. Using both conventional and transient swelling hydraulic conductivity relationships, similar trends for the resaturation process were observed although some variations were observed in the buffer materials' degree of saturation.
profile. It is apparent that further simulations are needed to improve the understanding on the effects of swelling in the buffer zone, especially when heating is involved.

7.5 Thermal Hydraulic Simulation of the In-room Geometry

The following sections detail analyses of the thermal hydraulic performance of the In-room geometry. Numerical results from simulations that use the conventional and transient swelling hydraulic conductivity relationship are shown, and the differences between both approaches discussed.

7.5.1 Initial and Boundary Conditions

Having established a suitable domain size and sufficient discretisation to represent the heating response in the In-room geometry, the same mesh as shown earlier in Figure 7.5 was adopted for thermo-hydraulic simulations. The simulations performed fully couples the hydraulic field with thermal response of the system which arises from the heat energy produced by waste material.

The initial pore water pressure and boundary conditions applied are as previously used in the hydraulic analysis. Similarly, the initial and boundary conditions for temperature are as used in the thermal analysis. The lower bound heat flux for the canister was used in the simulations. Similar to the hydraulic simulation, both conventional and micro-macro transient swelling relationship were used for the thermal hydraulic simulations with the transient swelling model applied to the inner and outer buffer material. The backfill materials were not expected to display much swelling and have assumed a conventional hydraulic conductivity relationship.

A similar time stepping scheme as that prescribed for the thermal analysis was used for the analyses. Again both spatial and temporal convergence were checked. The thermal and hydraulic relationships for each material have been described earlier in Chapter 5.
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7.5.2 Numerical Results

The following sections present the numerical results for the temperature, moisture and suction distribution in the In-room geometry.

7.5.2.1 Temperature results

Figure 7.21 and Figure 7.22 present the transient temperature profile along the mid-line of the canister and transient change in the temperature simulated at pre-selected points in the emplaced materials. Similar trends were observed when compared with the thermal response simulated for the thermal analysis. However, an overall temperature increase was observed for the coupled thermal and hydraulic simulation. A peak temperature of 382 K was simulated at the canister's surface at 10 years, 6 K higher than the peak temperature simulated for the thermal-only analysis. The temperature difference between the canister's surface and the far field rock had also reduced from 55 K at 10 years, down to only 16 K at 100 years.

The coupling between thermal and hydraulic response was clearly affecting the temperature profile in the emplaced system. As the waste canisters heated up the emplaced system, moisture in the buffer materials was driven away from the canisters, resulting in a decrease in the degree of saturation. Consequently, the buffer materials' thermal conductivity was reduced leading to a build up of temperature, thus accounting for the greater temperature increase in the thermal hydraulic simulation (as compared to the response from the thermal simulation).

Temperature results obtained from the simulation using the proposed transient swelling relationship were found to yield similar results when compared with those obtained from the earlier simulation (which used conventional hydraulic conductivity relationships for the emplaced materials). Hence, the results have not been presented here and are taken the same as those shown in Figure 7.21 and Figure 7.22.

7.5.2.2 Suction and Degree of saturation profile

In this section, the hydraulic responses obtained from the thermal hydraulic simulation using conventional hydraulic conductivity relationship are presented. Following that, numerical results obtained using the proposed transient swelling hydraulic relationship are also presented and discussed.
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Figure 7.23 presents the pore water pressure contour plots at various periods. In Figure 7.24 and 7.25, the transient degree of saturation profile along the midline of canister and the transient change in the degree of saturation in various pre-selected points are shown. It can be seen that comparisons between the suction and degree of saturation profile for the thermal hydraulic and isothermal hydraulic simulations indicate different trends. The coupling of the heating effect into the hydraulic response was clearly affecting the resaturation process and has extended the time needed to fully resaturate the emplaced system.

At the beginning of the simulation, the drying effect on the emplaced system was limited and the hydraulic gradients between adjacent materials were influencing the resaturation process. As the simulation progressed, the drying process gradually became more significant, particularly in the inner buffer near the waste canister. The decrease in the degrees of saturation in the emplaced materials was due to a vapour driven drying mechanism. The simulation results had also indicated that after 5 year, there was little transient change in the degree of saturation for the near field rock. This suggests that water was infiltrating steadily into the unsaturated emplaced system, whilst the saturated surrounding rock was continuously supplying water. The coupling between the thermal and hydraulic process has also developed a drying-wetting mechanism. The drying process in the buffer materials increased the suction value, thus creating a hydraulic gradient. Resultantly, water is drawn from the rocks. This mechanism in effect prevents a cyclic overheating.

As mentioned previously, the transient swelling hydraulic conductivity relationship developed in Chapter 6 was then applied in the thermal hydraulic analyses. Figure 7.26 and Figure 7.27 present the pore water pressure contour plots at various times and the degree of saturation profile along the midline of canister obtained using the transient swelling model. In Figure 7.28, the transient changes in the degree of saturation at different points along the midline of canister are presented.

Unlike the thermal responses, the degree of saturation and suction profiles obtained for the emplaced system differ significantly when compared with results attained using conventional hydraulic conductivity relationship. Observing Figure 7.27, the degree of saturation gradient across the inner and outer buffer material was higher.
Buffer materials in the emplaced system were also resaturating at a slower rate. The gradient differences are attributed to the swelling mechanism at the buffer/backfill interface. As the suction difference drew moisture towards the buffer material, the degree of saturation at the materials' interface approached saturation. Correspondingly, the swelling model yields a large decrease in the hydraulic conductivity. This represents a reduced capacity for free water movement and prevents moisture from entering the buffer materials easily.

The scenario was further aggravated by the temperature rise at the canister’s surface, driving moisture away from the buffer materials. Observing the degree of saturation at the dense and light backfill in Figure 7.24 and 7.27, the latter was much higher. The swelling simulated in the materials' interface has retarded the supply of moisture from the backfill materials, and resulted in a greater increase in the degree of saturation in these backfills. Temperature increase at the canister’s surface has also intensified the vapour pressure and worsened the drying process.

A complete resaturation was achieved at 120 years, 40 years later than that predicted using the conventional hydraulic conductivity relationship.

7.5.3 Conclusion

In the numerical simulations presented, both conventional and transient swelling adsorbed/free water hydraulic conductivity relationships have been applied. It can be seen that the pore water pressure and suction response in the analyses were significantly different. The incorporation of the proposed transient swelling hydraulic conductivity model resulted in similar effects to those observed in the Buffer/Container Experiment where the swelling effect was clearly affecting the resaturation process. The proposed model also indicated that complete resaturation of the emplaced system would take longer, and the buffer materials were drier compared to that suggested using the conventional flow relationship.

The In-room geometry is still a proposed layout with no field data to ascertain the accuracy of the simulated results. However, simulation results obtained using the proposed transient swelling hydraulic conductivity relationship delivered good correlations when compared with available measured data in the Buffer/Container
Experiment. In view of this, the author has decided to adopt the conceptual model which accounts for the swelling effects in the subsequent thermo/hydro/mechanical simulation for the proposed geometry.

7.6 Thermo/Hydro/Mechanical simulation for the In-room Geometry

7.6.1 Introduction

Having performed a coupled thermal hydraulic simulation for the In-room geometry, it is now logical to investigate the influence of swelling on the stress/strain behaviour of the system. Hence, a coupled thermo/hydro/mechanical analysis of the In-room geometry has been performed. The mesh shown earlier in Figure 7.5 was again employed to describe the domain. The initial and boundary conditions specified for the moisture and temperature flux in this model were identical to the conditions in the thermal hydraulic simulation described in Section 7.5. The time stepping scheme applied in the thermal analysis was again used in the simulation. The mechanical parameters for the emplaced materials and surrounding host rock in the analysis were taken from Chapter 5. Similar to the analysis of the Buffer/Container Experiment, the rock was restrained completely. The emplaced materials along the symmetry line were assumed restrained along the horizontal direction but free to slide along the vertical direction. All other boundaries were prescribed a condition of zero moisture and temperature flux. As there was no available information on the as-placed stress conditions of the emplaced materials, an initial uniform stress of 200 kPa was assumed for the materials. Again numerical checks were made to ensure convergence in the temporal and spatial fields.

The following sections present the numerical results for the temperature, moisture and suction distribution, as well as the stress/strain response and displacements predicted in the emplaced materials. Where appropriate, comparisons have been made against the numerical results obtained in the earlier thermal hydraulic simulations and are presented herein.
7.6.2 Temperature and moisture field

Figure 7.29 and Figure 7.30 present the temperature profile obtained along the midline of the canister and a comparison between the transient temperature change at the canister’s surface, light backfill and rock obtained from the thermal hydraulic and deformation analysis. Similar trends were observed for both sets of simulations with temperatures peaking at 10 years. However, the temperature profile at the canister’s surface (from the deformation analysis) indicated a slower rate of cooling, where temperature difference during the cooling down period was up to 15 K.

The numerical results obtained for the moisture profile are also shown in this section. Figure 7.31 and Figure 7.32 show the pore water pressure contour plots and the transient degree of saturation profile along the mid-line of the proposed layout. Figure 7.33 presents a comparison between the thermal hydraulic and deformation analysis results, showing the transient change in the degree of saturation at the canister’s surface and the near field rock, are presented.

Observing both Figure 7.31 and Figure 7.32, it can be seen that at the beginning of the simulation, the buffer materials were beginning to dry whilst water was infiltrating into the emplaced system from the surrounding saturated rock. The hydraulic response from the thermo/hydro/mechanical analysis was comparable with the thermal hydraulic simulation result. At the beginning of the heating phase, the temperature and suction effects on the deformation aspects of the In-room geometry were still limited. Similar to the thermal hydraulic analysis, the effect of swelling on the hydraulic conductivity was evident, particularly at the outer buffer and dense backfill interface. Despite the large increase in the degree of saturation (due to infiltration of moisture from the surrounding rock into the emplaced system) at the dense backfill, the moisture content level in the buffer materials remained low. The saturated micropores at the buffer-backfill interface has swelled up and as a result retarded the flow of moisture. Furthermore, the heating from the waste canisters has resulted in an increase of voids in the buffer materials. As a result, the degree of saturation in the buffer materials decreased even further.

The inclusion of deformation in the numerical model has also extended the time needed for the emplaced system to fully resaturate. Inspecting Figure 7.33, the rate of
resaturation in the buffer was significantly slower for the thermo/hydro/mechanical analysis. As discussed earlier, the thermal expansion in the heated materials has increased the volume of voids, thus intensifying the resaturation effort. The degrees of saturation at both ends of the canister are different in the analysis. This was due to the proximity of these selected points from the surrounding host rock, as well as the positioning of the waste canisters.

7.6.3 **Stress-strain behaviour in the emplaced materials**

In this section, the stress and strain results from the thermo/hydro/mechanical analysis are presented. Figure 7.34 and Figure 7.35 present the horizontal stress profiles along the midline of canister and a vertical section 0.1 m away from the symmetry line. In Figure 7.34, the stress profiles at each period shared the same trend. The stress build up in the buffer materials between the canisters was found to be lower than other parts of the In-room materials. Both thermal expansion and moisture inflow from the rocks have contributed to the pressure build up in the emplaced system. The difference in pressure build up in the buffer materials during the initial stages was due to the lower density backfill materials absorbing the stress increase from the adjacent buffer materials. As the simulation progressed, the large stress build up in the buffer materials near the symmetry line began to dissipate away.

In Figure 7.35, the stress build up in the rock was significantly higher than the stress in the emplaced materials. As the rock was totally restrained, the temperature increase in the rock was not able to generate any material expansion. Consequently, the stress build up could not be relieved. Horizontal stress near the buffer-backfill interface was significantly higher. As mentioned earlier in Section 7.6.2, swelling was simulated at the interface. This would induce further stress increase near the materials' interface.

The vertical stress profiles are also presented in this section. Figure 7.36 and Figure 7.37 present the vertical stress profiles along the midline of the canister and at a vertical section 0.1 m away from the symmetry line. Stress profiles at the inner buffer indicated an increase in vertical stress at the early stages of the simulation. However, the stress build up was later absorbed by the outer buffer and backfills. In Figure 7.37, a similar trend as that observed for the horizontal stress profile was obtained.
The void ratio profiles simulated for the In-room geometry are presented in Figure 7.38 and Figure 7.39 respectively. Void ratio at the inner buffer was predicted to change significantly. During the early stages, void ratio near the inner and outer buffer interface was increasing due to moisture inflow and the drying effect near the canister. However, as the simulation continued, void ratio in the inner buffer began to decrease. The thermal shrinkage and material expansion in the backfill materials have resulted in the overall decrease in void ratio in the inner buffer.

7.6.4 Conclusions

A coupled thermo/hydro/mechanical analysis has been performed to investigate the effects of including deformation in the simulation of the repository’s performance. Comparisons between results obtained from the thermal hydraulic and the deformation analysis showed a number of differences. The inclusion of deformation in the numerical model has prompted a greater drying effect and also delayed the rate of resaturation in the emplaced system. The system was predicted to take longer to fully resaturate. Although some of the deformation parameters employed in the deformation analysis have been based on various assumptions, this study has demonstrated the effects deformation can have on a typical horizontal canister deposition configuration, thus providing a better indication on the performance of an actual experiment.

7.7 Thermal-Hydraulic Simulation of the In-room Geometry in Saline Conditions

Under saline conditions, saturated hydraulic conductivity values for the emplaced materials can be up to three orders of magnitude higher than those under freshwater conditions. In view of this, the performance of the In-room geometry under saline conditions was investigated. The following sections set out to describe the numerical results obtained. The differences between the response in freshwater and saline conditions are also discussed and presented.
Chapter 7  Simulation of a Horizontal Canister In-room Emplacement Configuration

7.7.1  Initial and Boundary Conditions

Initial and boundary conditions as described in Section 7.5.1 were applied for the thermal hydraulic simulation in saline conditions. The transient swelling hydraulic conductivity relationship was used in the numerical model. The thermal conductivity relationship for each emplaced material remained unchanged. However, the saturated hydraulic conductivities for the emplaced materials were altered to values obtained under saline conditions (Dixon et al., 2002).

7.7.2  Numerical Results

Temperature results for the In-room geometry under saline conditions simulation are presented in Figure 7.40 and 7.41. Compared with temperature results obtained for freshwater conditions, similar trends were observed. Figure 7.41 indicates that the peak temperature obtained at the canister's surface was 375 K, 7 K lower than that achieved in freshwater conditions. Temperatures in the backfill and surrounding rock gave results that closely matched those obtained in the freshwater simulation.

Figure 7.42 shows the pore water pressure contour plots at various stages for the thermal hydraulic analysis in saline conditions. Compared with the response obtained for freshwater conditions (shown in Figure 7.26), it can be seen that the emplaced materials were registering lower suction values. This was due to the higher hydraulic conductivity in the emplaced materials, thus facilitating a faster rate of infiltration into the emplaced system. Figure 7.42 indicates that at 3 years and 10 years, a significant pore water pressure difference between the concrete layer and the dense backfill was simulated. The positioning of the concrete at the base of the proposed horizontal deposition configuration has affected the moisture inflow from the host rock into the dense backfill. Consequently, a pore water pressure build up was predicted at the base of the placement. However, the pressure build up soon dissipated.

Figure 7.43 and 7.44 present the transient degree of saturation profile along the midline of canister and the transient change in the degree of saturation at various materials. With the exception of the inner buffer, the degree of saturation profile for
each emplaced material was near constant. Observing Figure 7.44, it can be seen that the inner buffer had begun resaturating after 3 years.

Similar to the response simulated for the thermal hydraulic analysis in freshwater conditions, the resaturation process was driven primarily by the hydraulic potential between the emplaced materials and rocks, as well as the evaporation-condensation cycles. However, unlike the intensity of drying observed in the freshwater simulation, the decrease in moisture content in the buffer materials was much less in saline conditions. In saline conditions, the rate of flow in the emplaced materials was considerably higher, thus favouring the resaturation processes in the unsaturated buffer and backfill materials.

The hydraulic and temperature responses obtained in freshwater and saline water conditions have been compared and found to vary in many aspects. In freshwater conditions, the evaporation process dominated over the condensation process. Higher suction values were observed in the buffer and backfill materials, particularly near the heat source. On the contrary, in saline conditions the resaturation processes were dominant. In addition, peak temperature predicted at the canister's surface was considerably lower and the engineered materials' degree of saturation was higher, when compared with the freshwater analysis.

7.7.3 Conclusions

The simulation for In-room geometry in saline conditions has highlighted several critical differences when compared with results from the freshwater simulation. The temperature increase at the canister's surface was much lower in saline conditions. Also, the rate of water uptake in the emplaced materials was found to be faster, thus facilitating a complete saturated state in the In-room at an earlier time. The simulated results obtained have also indicated that as the overall permeability of the emplaced system was increased, the drying effect in the buffer materials as well as the swelling phenomena became less pronounced in the In-room geometry.
7.8 Sensitivity Analysis on the Threshold Pressure Parameter for the In-room Geometry Simulation (Thermal-Hydraulic)

7.8.1 Introduction

Threshold pressure for granite rocks has been determined via the approach described in Section 5.2.2 where Davies (1991) was reported to have defined threshold pressure as being "the gas pressure required to overcome capillary resistance that will lead on to outward gas flow". In other words, the threshold pressure parameter used in the simulation of the In-room geometry would affect the water retention curve, and consequently influence the rate of water uptake from the rock region. Simulations of the Buffer/Container Experiment reported in Chapter 6 have demonstrated the important role of the buffer-rock interaction, in particular its influence on the resaturation process in the disposal layout.

As mentioned previously, the threshold pressure affects the rate of infiltration of water from the surrounding host rock into the emplaced system. Due to a lack of experimental data to ascertain the actual value of the threshold pressure, research results obtained from Davies (1991) which correlated the relationship between threshold pressure and intrinsic permeability, was used to determine an averaged entry value. The author decided to investigate the effects of adopting a higher and lower bound threshold value on the excavation damaged zone (EDZ) and the granite rock in the simulation of the In-room geometry. The following sections present the predictions obtained and discusses the effect threshold pressure value has on the In-room geometry's performance.

7.8.2 Initial and Boundary Conditions

Initial and boundary conditions used previously in Section 7.5.1 for the thermal hydraulic analysis were applied to the high and low threshold pressure simulations. As stated previously, any undefined boundaries were automatically prescribed a condition of zero moisture and temperature flux. The thermal and hydraulic parameters for the emplaced materials remain unchanged, except for the threshold pressure adopted for inner EDZ, outer EDZ and host rock. The transient swelling
hydraulic conductivity model has also been incorporated into the numerical model. The upper and lower bound threshold pressure in these rock regions have been described in Chapter 5.

### 7.8.3 Numerical Results

The simulated temperature results for the upper and lower bound threshold pressure simulations showed little difference when compared with the response predicted using an averaged threshold pressure simulation. Hence, the temperature results will not be presented here.

Figure 7.45 and Figure 7.46 illustrate the pore water pressure contour plots for the upper and lower bound threshold pressure analysis. It can be seen that the pore water pressure in the far field rock for the lower bound simulation was much higher than for the upper bound threshold pressure analysis. The contour plots at 100 years for both sets of analyses indicated that the In-room geometry was fully saturated.

Figure 7.47 and Figure 7.48 present the degree of saturation profiles along the mid-line of canister and the transient change in the degree of saturation at various points representing different emplaced materials. Comparison between both sets of analyses shows that a similar trend was predicted for the hydraulic response. As the water retention curve adopted for the rock in each simulation was dependent on the adopted threshold pressure, the initial suction assumed in the unsaturated rock for both simulations were also different. Observing Figure 7.48, the rate of resaturation simulated in the rocks was visibly slower for the lower threshold pressure simulation. The moisture retention curve for the rock adopting a lower threshold pressure resulted in water permeating through with less difficulty, thus allowing a faster rate of resaturation.

### 7.8.4 Conclusions

Sensitivity analyses on the threshold pressure parameter have indicated some differences in the suction profile of the In-room geometry. A higher threshold pressure in the rocks would increase the rate of resaturation in the rock region.
7.9 Influence of Hydrostatic Pressure on the Performance of In-room Geometry

7.9.1 Introduction

So far, the simulation works performed on the In-room geometry have been conducted based on the assumption that the depth of placement was at 500 m below ground level. The hydrostatic pressure, at which the emplaced materials were subjected to, would affect the hydraulic gradient imposed on the emplaced system and consequently the rate of water uptake. Personal communication with AECL (2002) indicated that the proposed In-room geometry was likely to be located between 500 m and 1000 m deep. Hence, further investigation was needed to assess the effects of hydrostatic pressure and its influence on the thermal and hydraulic responses in the proposed layout. The following sections present predictions obtained at 500 m, 750 m and 1000 m below ground level, as well as evaluating the influence hydrostatic pressure has on the In-room geometry’s performance.

7.9.2 Initial and Boundary Conditions

The mesh shown earlier in Figure 7.5 was again used to simulate the In-room geometry at 750 m and 1000 m deep. The initial suction values adopted for the emplaced materials in the earlier thermal hydraulic analysis were used in the analyses. However, the initial pore water pressure for the far field rock was prescribed its corresponding hydrostatic pressure. For example, rock at mid-line level of the repository was prescribed pore water pressure values of 7.36 MPa and 9.81 MPa at 750 m and 1000 m below ground level respectively. Following the approach taken for the earlier thermal hydraulic analysis (shown in Section 7.5.1), the water pressure was gradually decreased through the near field rock, down to 0 Pa at the tunnel surface. Far field boundaries were fixed at their initial temperature and pore water pressure values. The thermal and hydraulic parameters used the same parameters as described in Chapter 5. The transient swelling hydraulic conductivity relationship was again applied in the model. As before, all non-prescribed boundaries were given a condition of zero moisture and temperature flux normal to the boundary surface. The time-stepping scheme used previously in the initial thermal hydraulic simulation was employed in the numerical model.
7.9.3 Numerical results

Figure 7.49 and 7.50 demonstrate the transient temperature profile along the mid-line of canister and the evolution of the simulated temperature at the canister’s surface and near field rock. Looking at Figure 7.49, a similar trend was observed. Temperatures simulated at 10 years for the buffer material at 1000 m depth was found to be lower than the temperatures simulated at 500 m and 750 m depth. For a 1000 m deep repository, a higher potential gradient would increase the rate of water uptake into the emplaced system. Consequently, thermal conductivity for the emplaced materials would increase, thus allowing the generated heat near the canister to dissipate more readily. Figure 7.50 also indicates that materials further away from the heat source for all three analyses have similar temperature variations.

Figure 7.51 and Figure 7.52 present the pore water pressure contour plots for the In-room geometry at 750 m and 1000 m respectively. Similar plots at 500 m depth are displayed in Figure 7.26. Contour plots produced for the suction field at 1000 m depth suggest that water infiltration from the surrounding rock was much faster compared to the other two analyses. Pore water pressure plots at 100 year indicate that only the 1000 m deep analysis was not completely resaturated.

The degree of saturation profiles along the mid-line of the repository at half year, 10 years and 40 years are illustrated in Figure 7.53, Figure 7.54 and Figure 7.55 respectively. At 6 months, it can be seen that the rate of resaturation in the rock was slowest at 500 m depth and fastest at 1000 m depth. The degree of saturation profiles presented at 500 m and 750 m depths, were similar in the buffer and backfill regions. At 1000 m deep, the higher hydrostatic pressure exerted by the surrounding host rock was able to increase the rate of water uptake. Consequently, the level of the degree of saturation in the emplaced materials would further increase the materials’ thermal conductivities, thus allowing heat to disperse more efficiently. The degree of saturation profiles in the buffer materials for the analyses were found to be uneven. As discussed earlier, this was due to a larger resource of moisture provided by the adjacent backfills and rocks.

Figure 7.56 details the simulated transient degree of saturation profiles at the canister’s surface and inner EDZ at depths of 500 m, 750 m and 1000 m depths. The
analyses suggested an immediate resaturation occurring in the rock. It was also observed that as the depth of placement increases, the time taken for the rock to fully resaturate was shortened.

At the canister’s surface, the analyses showed a significant amount of drying before recovering back to full saturation. As the emplaced materials were heated up, the evaporation process was driving moisture away from the canister. As a result, high suction was developed in the inner buffer. The suction imbalance resulted in moisture being drawn from the surrounding wet rocks. However during resaturation, the condensation process began to take precedence over the evaporation process. This was further intensified by the cooling in the waste canisters.

Complete resaturation was initially attained at 750 m depth, followed by 1000 m and finally at 500 m depth. In the 1000 m depth analysis, the accelerated arrival of moisture into the emplaced materials, particularly at the buffer/backfill interface, resulted in swelling during the early stage. Accordingly, the flow into the buffer materials became retarded, thus hindering the resaturation in the buffer materials and extending the time needed to achieve complete resaturation for the In-room geometry.

7.9.4 Conclusions

An investigation into the effect of hydrostatic pressure on the performance of the In-room geometry has been performed. It was found that the depth of placement for a repository yielded a significant impact on the hydraulic and thermal responses of the In-room geometry. As the depth of placement was increased, the temperature increase observed in the emplaced system, particularly for the buffer materials became less apparent. The swelling effect which was included in the analyses was also found to affect the rate of water uptake simulated in the emplaced system.

7.10 Conclusion

The complex geometry layout for the In-room geometry has presented a challenge for simulation purposes. Despite the lack of experimental data, the materials’
relationship assigned for the simulation of the In-room geometry is thought to be representative of the actual material itself.

A thermal-only analysis, an isothermal hydraulic analysis, followed by a thermal hydraulic analysis was systematically carried out before arriving at a fully coupled thermo/hydro/mechanical analysis of the In-room geometry. Several primary factors thought to affect the In-room geometry’s performance have been identified. These include the heat output from the waste canisters; the hydraulic potential gradient between the emplaced system and the surrounding rock; and the placements of various engineered-materials with different soil properties.

Similar for the Buffer/Container Experiment, the transient swelling hydraulic conductivity model was applied in the In-room geometry. The simulated results had indicated that swelling at the buffer materials' interface has intensified the drying process and affected the rate of water uptake from the rocks. Shrinkage was also simulated near the heater. As mentioned previously, although no field data is available to verify the analyses results, the simulated responses achieved using the transient swelling model are thought to be reasonable.

Sensitivity analyses on critical material parameters have yielded indicative insights on several hypothetical scenarios. Under saline conditions, the hydraulic conductivities for the emplaced materials would increase by several orders. Consequently, the rate of resaturation would be increased, thereby reducing the time taken to achieve complete saturation. The increase in degree of saturation in the emplaced materials would also increase the overall thermal conductivity of the system, thus resulting in a lower temperature increase at the canister’s surface.

The variation of the threshold pressure value in the rock has affected the In-room’s hydraulic performance. The rate of resaturation in the rock was much faster when a higher threshold pressure value was adopted. A threshold pressure change would change the moisture retention curve, thus affecting the resaturation processes. The analyses indicate that a proper characterisation of the surrounding rocks’ ability to supply water into the emplaced system is necessary.
Sensitivity analyses on the hydraulic potential imposed upon the emplaced system showed a significant impact on the repository's performance. As the In-room was lowered to a greater depth, the hydrostatic pressure would increase. Moisture would infiltrate faster into the In-room and the rate of resaturation in the emplaced system would be increased. This suggests that careful consideration is required when determining the actual location of the In-room geometry.

The sensitivity studies have provided valuable insights into the In-room system. Also, the analyses have demonstrated that the critical parameters identified have affected In-room's performance to varying degrees.

### 7.11 Reference


Table 7.1 Thermal properties and the hydraulic conductivity of each material

<table>
<thead>
<tr>
<th>Material</th>
<th>Thermal conductivity, W/m.K</th>
<th>Heat capacity, J/kg.K</th>
<th>Density, kg/m$^3$</th>
<th>Saturated hydraulic conductivity, m/s</th>
</tr>
</thead>
<tbody>
<tr>
<td>Copper container</td>
<td>380</td>
<td>390</td>
<td>8930</td>
<td>0</td>
</tr>
<tr>
<td>Inner buffer</td>
<td>0.3 (dry)</td>
<td>880 (dry)</td>
<td>1610 (dry)</td>
<td>5.0E-13***</td>
</tr>
<tr>
<td></td>
<td>0.95 (ap)</td>
<td>1290 (ap)</td>
<td>1840 (ap)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1.25 (sat)</td>
<td>1520 (sat)</td>
<td>2010 (sat)</td>
<td></td>
</tr>
<tr>
<td>Gap fill</td>
<td>0.3 (dry)</td>
<td>890 (dry)</td>
<td>1400 (dry)</td>
<td>1.0E-12**/</td>
</tr>
<tr>
<td>- Reference (100% pellets)</td>
<td>0.3 (ap)</td>
<td>910 (ap)</td>
<td>1410 (ap)</td>
<td>1.0E-11*</td>
</tr>
<tr>
<td></td>
<td>1.2 (sat)</td>
<td>1710 (sat)</td>
<td>1880 (sat)</td>
<td></td>
</tr>
<tr>
<td>Gap Fill</td>
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<td>900 (dry)</td>
<td>1240 (dry)</td>
<td>1.0E-11**/</td>
</tr>
<tr>
<td>- Alternative (50:50 mixture)</td>
<td>0.7 (ap)</td>
<td>1280 (ap)</td>
<td>1400 (ap)</td>
<td>1.0E-9*</td>
</tr>
<tr>
<td></td>
<td>1.4 (sat)</td>
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<td>1780 (sat)</td>
<td></td>
</tr>
<tr>
<td>Outer buffer (50:50 mixture)</td>
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<td>870 (dry)</td>
<td>1690 (dry)</td>
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<td>1350 (ap)</td>
<td>1980 (ap)</td>
<td>1.0E-10+</td>
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<td></td>
<td>1.7 (sat)</td>
<td>1460 (sat)</td>
<td>2060 (sat)</td>
<td></td>
</tr>
<tr>
<td>Dense backfill (5:25:70 mixture)</td>
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<td>860 (dry)</td>
<td>2120 (dry)</td>
<td>2.0E-11**/</td>
</tr>
<tr>
<td></td>
<td>2.0 (ap)</td>
<td>1100 (ap)</td>
<td>2280 (ap)</td>
<td>2.0E-11*</td>
</tr>
<tr>
<td></td>
<td>2.0 (sat)</td>
<td>1160 (sat)</td>
<td>2330 (sat)</td>
<td></td>
</tr>
<tr>
<td>Light backfill (LBF)</td>
<td>0.5 (dry)</td>
<td>900 (dry)</td>
<td>1240 (dry)</td>
<td>1.0E-11**/</td>
</tr>
<tr>
<td>- Reference (50:50 mixture)</td>
<td>0.7 (ap)</td>
<td>1280 (ap)</td>
<td>1400 (ap)</td>
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<td>1.4 (sat)</td>
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<td>1400 (dry)</td>
<td>1.0E-12**/</td>
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<tr>
<td>- Alternative (100% pellets)</td>
<td>0.3 (ap)</td>
<td>910 (ap)</td>
<td>1410 (ap)</td>
<td>1.0E-11*</td>
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<tr>
<td></td>
<td>1.2 (sat)</td>
<td>1710 (sat)</td>
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<tr>
<td>Concrete (LHHPC)</td>
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<td>2430</td>
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<td>EDZ rock – inner 0.30 m</td>
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<td>1.0E-10</td>
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<tr>
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<td>Host rock</td>
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<td>845</td>
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</tr>
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</table>

** Value based on freshwater conditions

+ Value based on 100g/L saline conditions
Table 7.2  Initial porosities and degree of saturation of materials (as-placed)

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<tr>
<th>Material</th>
<th>Initial porosity</th>
<th>Initial degree of saturation</th>
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<tbody>
<tr>
<td>Container</td>
<td>0</td>
<td>n/a</td>
</tr>
<tr>
<td>Inner buffer</td>
<td>0.41</td>
<td>60</td>
</tr>
<tr>
<td>Gap fill (50:50)</td>
<td>0.55</td>
<td>33</td>
</tr>
<tr>
<td>Gap fill (100%)</td>
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<td>6</td>
</tr>
<tr>
<td>Outer buffer</td>
<td>0.38</td>
<td>80</td>
</tr>
<tr>
<td>Dense backfill</td>
<td>0.22</td>
<td>80</td>
</tr>
<tr>
<td>Light backfill (50:50)</td>
<td>0.55</td>
<td>33</td>
</tr>
<tr>
<td>Light backfill (100%)</td>
<td>0.49</td>
<td>6</td>
</tr>
<tr>
<td>EDZ rock inner</td>
<td>0.006</td>
<td>Varies</td>
</tr>
<tr>
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<td>Varies</td>
</tr>
<tr>
<td>EDZ notch</td>
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<td>Host rock - near-field</td>
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<td>Host rock - far-field</td>
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<td>100</td>
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<tr>
<td>Concrete**</td>
<td>0.15</td>
<td>50</td>
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</table>

Table 7.3  Variation of container heat output with time

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<th>Time (years)</th>
<th>Reduced power (W)</th>
<th>Full power (W)</th>
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<tr>
<td>0</td>
<td>890</td>
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<tr>
<td>10</td>
<td>759</td>
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<tr>
<td>9960</td>
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<td>44.5</td>
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Figure 7.1  A three-dimensional illustration of the In-room geometry (extracted from OPG, 2001)
Figure 7.2 Layout of a typical cross-section of the In-room geometry
Figure 7.3  Plan layout of the In-room geometry
Figure 7.4 Layout of emplaced materials for the In Room Geometry
Figure 7.5  (a) Full mesh

(b) Detailed mesh in tunnel
Canister containing decaying high level nuclear waste material (rate of decay described by Tait et al., 2000)

Uniform initial temperature of 286K

Temperature fixed at 286 K

All other boundaries have zero flux

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Chapter 8

Conclusions

8.1 Introduction

This chapter sets out to report on the conclusions from the investigations carried out. Suggestions for further research work are also presented later in the chapter.

Earlier in Chapter 1, the main objectives for this study were defined and are shown as follow:-

- To review the developments made in the modelling of high level nuclear waste repositories and investigate the influence of the micro-macro structure of clay on moisture flow in an engineered buffer material.

- To develop and implement a conceptual model capable of describing the effects of swelling phenomena on the behaviour of buffer materials.

- To investigate the thermo/hydro/mechanical interaction between an unsaturated buffer material and a saturated rock, under the effects of thermal and hydraulic potential gradients.

- To predict the thermal, hydraulic and mechanical response for a horizontal canister deposition configuration.

- To investigate the influence of material parameters on a repository’s performance and improve the understanding on the thermal/hydraulic interactions between rock and clay barrier.
It is claimed that each of the objectives listed above have been achieved. The following sections detail the conclusions from the study carried out.

8.2 Review of the developments in the modelling of high level nuclear waste repositories and the effects of micro-macro structure on moisture flow

A review into available literature shows that much research work has been performed on the development of the concept of underground waste repositories. The configuration of engineered buffer materials and natural barrier systems, as well as the compatibility of the soil components in a repository layout has received considerable attention from researchers all over the world. Experimental studies of varying scales, ranging from small scale bench top experiments to large scale in situ experiments have been conducted. The results from these experiments have been used to validate numerical models, thus enhancing the ability of these models to predict the performance of underground waste repositories. A good example is the Buffer/Container Experiment, which was performed by the AECL. As a comprehensive large scale in situ experiment, it was set up to examine the effects of heating on the clay buffer and presents an opportunity for scientists to test their numerical models.

Increasingly, investigations have also been performed to link the microscopic characteristics of clay-based buffer material to its macroscopic behaviour. Researchers recognise the importance of achieving reasonable compatibility between the conceptual and the numerical models. A review carried out on moisture flow in unsaturated soil indicates that under the influence of physico-chemical forces that exist in the microstructure of clays, water found in the micropores behaves differently from water found elsewhere. This would affect moisture flow in swelling clay, especially when the soil is restrained from expanding.

8.3 Thermo/hydro/mechanical interaction between an unsaturated buffer material and a saturated rock

A comprehensive set of experimental results was obtained for AECL's Buffer/Container Experiment (Graham et al., 1997). The primary aim of the
experiment was to examine the effects of heating on the performance of the dense sand-bentonite buffer and the saturated granite rock in a typical vertical borehole configuration. A series of numerical analyses were performed and the simulation results have been compared with the experimental results.

Prior to analysing the heating phase, the pre-heating phase was modelled. This was necessary to ensure the conditions in the granite rock at the beginning of the heating phase were representative.

A coupled thermal hydraulic analysis of the heating period produced a good correlation between the simulated temperature results and the experimentally measured temperature change. It was concluded that the thermal behaviour was well represented in the numerical model.

A traditional hydraulic conductivity curve was assumed for the buffer material in the numerical analysis. However the simulated hydraulic profile did not give a good correlation with the experimental data. It was postulated that the experiment results indicated that swelling in the buffer near the host rock was affecting the moisture flow. It was concluded that the relationship between the microstructure and macrostructure had not been fully accounted for, and should be incorporated into the numerical model. It was found that a transient form of free/adsorbed water model gave the closest representation of the experimental results. The model will be discussed in detail in Section 8.4.

A coupled thermo/hydro/mechanical analysis was performed to investigate the deformation behaviour in buffer material. Good overall correlation was achieved when compared with the experimentally measured results. When the heater was activated, drying in the buffer close to the heater resulted in shrinkage. Moisture was also infiltrating into the buffer from the surrounding rock, causing swelling to occur in the buffer adjacent to the granite rock. Similar trends were observed for both the simulated and measured stresses. The numerical results for horizontal and vertical stresses were much higher than the experimental results. It was concluded that the buffer material in the actual experiment may have expanded into the cracks in the rock, thus relieving the pressure build up in the buffer material.
The overall good correlations achieved between the experiment and numerical results have increased confidence that the numerical model is capable of simulating the thermal, hydraulic and mechanical response in a swelling buffer material.

8.4 Conceptual modelling of the swelling phenomena in buffer material

Following investigations on a number of approaches, a conceptual model describing the swelling behaviour of a confined bentonite-based clay buffer material has been developed. Initially, an approach proposed by Mitchell (2002) was assumed for the numerical model. The proposed conceptual model incorporates an exponential relationship to describe the swelling behaviour of buffer material as it approaches saturation. However, the swelling model was unable to provide good correlation between the experimental results and the numerically simulated results. Further review indicated that water infiltrating through the buffer-rock interface might not be adsorbed immediately. It was concluded that a time dependent relationship that describes the adsorption and desorption of water at micropores, would better represent the swelling phenomena observed in the Buffer/Container Experiment.

The relationship was extended for a coupled thermo/hydro/mechanical relationship. The extent of the swelling effect depended on the level of restraint imposed on the buffer material. If the material was completely restrained, the overall void ratio would remain unchanged and any swelling in the micropores would result in a compression in the macropores. However, as the buffer material in the experiment was partially restrained, the reduction in the rate of flow would be much lesser. The deformation analysis incorporating the proposed micro-macro transient flow model provided a good correlation with the experimental results.

8.5 Thermo/hydro/mechanical response for a horizontal canister deposition configuration

The In Room Emplacement geometry was proposed by AECL as a potential design concept for a horizontal canister deposition configuration. The concept was seen as a viable alternative to a vertical borehole configuration such as the Buffer/Container Experiment.
A systematic numerical modelling approach was adopted to produce a coupled thermo/hydro/mechanical analysis of the In Room Emplacement. Initially, a thermal analysis was undertaken to investigate the thermal response in the emplaced system.

An isothermal hydraulic simulation was then carried out to investigate the resaturation for the proposed layout in the absence of any thermal effects. Both the conventional hydraulic conductivity relationship and the transient micro-macro swelling relationship used in Chapter 6 were employed in the model.

A coupled thermal hydraulic analysis was performed to investigate the heating effects on unsaturated emplaced materials and saturated host rock. The inclusion of the micro macro water transfer model was shown to lengthen the time required for complete resaturation and produce a more intense drying effect near the heater.

A coupled thermo/hydro/mechanical analysis of the In Room Emplacement was then conducted. Although no comparison against experimental data was possible, it was believed that the numerical model produced sensible results. As the waste canisters began to heat up, temperature near the canister increased and moisture was driven away from the heat source. The hydraulic gradient which exists between the saturated rock and the unsaturated emplaced materials was found to draw water from the rock. Swelling occurred at the buffer-backfill interface as it neared saturation. Consequently, the rate of flow was reduced and affected the resaturation process. As the waste canisters’ heat flux began to decrease, the drying effect decreased and the resaturation processes began to dominate.

On the deformation side, shrinkage was observed near the heater and swelling occurred as water began to infiltrate into the drier region. After the temperature had peaked, resaturation in the emplaced system resulted in a gradual pressure build up.

8.6 Sensitivity analysis on material parameters and assessing their influence on the buffer-rock interaction

Several sensitivity analyses have been performed on key parameters thought to affect the performance of the repository set-ups. In particular the influence these parameters have on the buffer-rock interface was analysed.
For the Buffer/Container Experiment, an investigation was undertaken to assess the buffer material’s saturated hydraulic conductivity. It was found that using a buffer material with low permeability, the swelling at the buffer-granite interface became more pronounced and the drying effect was greater in the buffer near the heater. In addition, a higher pressure build up was observed in the near field rock.

The influence of microstructure on the rate of vapour flow was also investigated. It was found that as the available area for vapour transfer was reduced, the drying processes were restricted and this consequently affected the resaturation process. However, as the simulation progressed and the buffer materials began to resaturate, the influence of vapour transfer on the repository’s performance began to reduce.

In the In Room Emplacement, freshwater conditions were replaced by saline conditions in the emplaced system. By imposing this condition and thereby resulting in increased hydraulic conductivities, the rate of water uptake was found to increase, thus greatly reducing the time needed for complete resaturation. There was much less drying in the emplaced materials and the peak temperature simulated at the surface of the waste canisters was also much lower.

The threshold pressures assumed for the rock materials were also varied. It was concluded that this parameter which affects the rate of water infiltration from the rock, has little effect on the emplaced buffers but significantly alters the rate of resaturation in the rocks itself.

The depth of placement for the emplacement was investigated by varying the hydrostatic pressure imposed onto the emplaced system. It was found that as the hydrostatic pressure was increased, the temperature rise in the emplaced materials was reduced. An increase in the hydraulic potential gradient allowed the unsaturated emplaced system to draw moisture more readily and reduce the effect of microscopic swelling in the buffer materials.

8.7 Overall Conclusions

Based on the simulation works that have been carried out on the Buffer/Container Experiment and the In-room geometry, several main conclusions can be drawn from
the simulated results. The numerical works described in Chapter 6 have shown that a traditional form of hydraulic conductivity relationship (such as the Green and Corey (1971) approach) was not able to describe the swelling effect in the buffer, and as a result incapable of correctly simulating the moisture redistribution in the buffer materials. Subsequent investigations have indicated that a transient swelling hydraulic conductivity relationship that attempts to correlate changes at microscopic level with the corresponding macroscopic responses was able to produce simulation results which measured up well against the experimental data sets. This shows that swelling was affecting the resaturation effort in the Buffer/Container Experiment, and that the relationship between micro-macro structures in a clay-water system needs to be addressed adequately to produce good simulation results. In addition, studies have also suggested that choking does not occur immediately and swelling in the clay-based buffer materials is time dependent.

Studies on the sensitivity of the Buffer/Container Experiment to parametric variations have also been carried out. The inherent permeability assigned to the buffer material was found to yield a considerable impact on the performance of the experiment. An increase in the buffer’s permeability would lessen the significance of swelling effect in the experiment. In addition, studies have shown that careful consideration is required to describe vapour velocity in the buffer. Existing vapour diffusion terms may require further adaptation to account for the influence of microstructure on vapour flow in clays.

The geometry layout for the In-room emplacement design was considerably more complicated than the Buffer/Container Experiment. An accurate set of physical parameters and material relationships are required in the numerical model to correctly predict the In-room geometry’s responses. Similar to the Buffer/Container Experiment, the interactions between adjacent materials were found to significantly affect the simulation results. As such, careful consideration is required to select appropriate buffer and backfill materials, so that the performance of the actual experiment can be optimized. However, as a proposed design, no experimental data sets exist. Hence, material relationships that were thought to be representative have been adopted in the numerical model. The simulated results were found to be realistic and can be assumed to provide an indicative response of an actual In-room
experiment. The resaturation processes in the emplaced materials were primarily driven by heating in the canisters and water infiltration from the surrounding rocks.

Sensitivity analyses on the In-room geometry have shown that the salinity of groundwater affects the rate of water uptake in the emplaced system. In saline condition, the overall permeability of the emplaced system increases and consequently reduces the effects of drying and swelling. The performance of the In-room geometry was also found to be affected by the threshold pressure changes in the rocks. The depth of placement for the In-room affects the geometry layout’s performance considerably. An increase in depth would result in a greater rate of water uptake and a lower increase in temperatures near the canisters.

8.8 Suggestions for further research

The proposed model has been shown to be capable of describing the thermal, hydraulic and mechanical response of a large scale, in situ experiment as well as producing reasonable predictions for a proposed experimental layout. However, the numerical code is under constant development and the following presents suggestions for further research works.

The transient free/adsorbed water transfer model used in this work to describe the swelling phenomena of the bentonite buffer could be further researched and improved. The relationship between free water and adsorbed water could be further investigated. The rate of adsorption and desorption could be determined via direct experimental tests. As the presence of clay in buffer or backfill materials can vary significantly, tests could be designed to investigate the degree of swelling in these materials.

Experimental work is also required to investigate the hydraulic response in bentonite-based materials near saturation under varying degrees of confinement. The experimental results could be used to validate the swelling model proposed in this study and widen its nature of application.

The numerical analyse performed on the Buffer/Container Experiment and the In Room Emplacement were both two dimensional formulation. A three dimensional formulation would provide a more representative simulation for a more complex
repository set up involving an array of boreholes. Further research on ways to reduce the computational time required to simulate complex meshes would also be beneficial.

Further experimental work is necessary to investigate the heating effect on vapour transfer process in clay soil samples. The outcome from this study could determine the level of influence micropores have on the overall response, thus improving the existing formulation used to describe vapour transfer.

8.9 Reference

