Contractor Report to RWM
FEBEX-DP: THM modelling

March 2017
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Preface

Radioactive Waste Management (RWM) carries out Research and Development (R&D) in support of geological disposal of the UK’s higher activity radioactive waste. The work presented in this report forms part of our R&D programme and was carried out on our behalf by Quintessa working as a contractor to Amec Foster Wheeler. The work has been reviewed by RWM and by two independent peer reviewers. RWM accepts the data and conclusions in this report.
FEBEX-DP: THM modelling

Quintessa’s contribution on behalf of RWM

Kate Thatcher

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Abstract

The FEBEX experiment at the Grimsel Test Site in Switzerland was an in situ full-scale Engineered Barrier System (EBS) test performed under natural resaturation conditions. Two simulant waste containers containing heating elements were emplaced in a tunnel in granitic host rock and were surrounded by FEBEX bentonite. The first Heater was removed from the experiment after 5 years of heating, and the second Heater was removed in 2015 after 18 years of heating, which made FEBEX the longest running experiment of its scale. The FEBEX-DP project completed dismantling of the FEBEX experiment in August 2015, having excavated Heater 2 and associated bentonite.

The work reported here uses data from the FEBEX in situ experiment and data from supporting laboratory work to continue development of coupled numerical models of the thermal, hydraulic and mechanical processes that control the behaviour of bentonite buffers in geological disposal facilities. Previous work for RWM developed an HM model, called the Internal Limit Model (ILM), for an MX-80 bentonite and sand mixture. The work herein documents the first application of this model to an alternative bentonite, and tests whether the model is transferable.
Summary

The FEBEX experiment at the Grimsel Test Site in Switzerland was an in situ full-scale Engineered Barrier System (EBS) test performed under natural resaturation conditions. The FEBEX experiment was based on the Spanish reference concept for spent fuel disposal in crystalline rock in which waste containers are placed horizontally in drifts and surrounded by a clay buffer constructed of highly-compacted bentonite blocks. In the FEBEX experiment, two simulant waste containers containing heating elements were emplaced in a tunnel in granitic host rock and were surrounded by FEBEX bentonite. FEBEX bentonite (also known as Serrata clay) comes from the Cortijo de Archidona deposit in Serrata de Nijar, Almeria, Spain and has a high montmorillonite content, large swelling pressure and low permeability. FEBEX was initiated and led by Enresa in 1995; heating started in 1997. The system was heavily instrumented with a total of 632 sensors installed in the bentonite and in the surrounding rock. A partial dismantling and sampling of the EBS was carried out during 2002 (FEBEX II), removing Heater 1 and much of the associated FEBEX buffer. Heater 2 was maintained at approximately 100°C from 1997 until 2015, which made FEBEX the longest running experiment of its scale. The FEBEX-DP project completed dismantling of the FEBEX experiment in August 2015, having excavated Heater 2 and associated bentonite.

Experimental data from the FEBEX programme provide an opportunity to develop coupled numerical models of the thermal, hydraulic and mechanical (THM) processes that control the behaviour of bentonite buffer in geological disposal facilities. In an ideal situation, models would be robust enough to be able to predict the safety critical behaviour of bentonite under conditions expected in a disposal facility.

RWM (Radioactive Waste Management) has instituted a wide-ranging project focusing on improving the understanding of thermal-hydraulic-mechanical-chemical (THMC) behaviour of bentonite buffers, which is being coordinated by Amec Foster Wheeler. The work reported here is one element under this wider project, focusing on the FEBEX experimental data, and represents an 18-month programme of work. Previous work for RWM (conducted in the DECOVALEX-2015 project) developed an HM model, called the Internal Limit Model (ILM), for an MX-80 bentonite and sand mixture which performed well in representing a range of laboratory and field scale tests. The work herein documents the first application of this model to an alternative bentonite, and tests whether the model is transferable. The previous work did not include thermal coupling, so this has been newly added and coupled to the hydraulic and mechanical models. Overall the ILM behaved better than expected given the differences in bentonite composition between the previous work and the FEBEX experiment and the need to include thermal effects.
Several smaller scale laboratory experiments have been modelled alongside the in situ test. The ILM model developed previously for MX-80 bentonite was calibrated across all the laboratory experiments and the in situ test rather than each experiment separately. This approach was adopted to explore the predictive power of the model. A consistent parameter set was found to represent almost all processes in the model, however permeability generally had to be calibrated separately for each experiment.

The data from the FEBEX in situ experiment have been used to investigate whether further updates to the ILM could resolve some of the outstanding discrepancies between the model results and the data. A proposed alternative representation resulted in an improved fit of the model data to the experimental data, and can be tested on a wider range of appropriate experimental data to determine its applicability outside of the FEBEX experiment.
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1 Introduction

The FEBEX (Full-scale Engineered Barriers Experiment, Lanyon and Gaus, 2013) experiment at the Grimsel Test Site in Switzerland consisted of an in situ full-scale Engineered Barrier System (EBS) test performed under natural conditions. The FEBEX experiment was based on the Spanish reference concept for spent fuel in crystalline rock in which waste containers are placed horizontally in drifts and surrounded by a clay buffer constructed of highly compacted bentonite blocks. In the FEBEX experiment, two simulant waste containers containing heating elements were emplaced in a tunnel through granitic host rock and were surrounded by FEBEX bentonite. FEBEX bentonite (also known as Serrata clay) comes from the Cortijo de Archidona deposit in Serrata de Níjar, Almeria, Spain and has a high montmorillonite content, large swelling pressure and low permeability (Lanyon and Gaus, 2013; ENRESA, 2000). FEBEX was initiated and led by Enresela in 1995; heating started in 1997. The system was heavily instrumented with a total of 632 sensors installed in the bentonite and in the surrounding rock. A partial dismantling and sampling of the EBS was carried out during 2002 (FEBEX II), removing Heater 1 and much of the associated FEBEX buffer (Lanyon and Gaus, 2013). Heater 2 was maintained at approximately 100°C from 1997 until 2015, which made FEBEX the longest running experiment of its scale. The FEBEX-DP project completed dismantling of the FEBEX experiment in August 2015, having excavated Heater 2 and associated bentonite (Lanyon and Gaus, 2013).

Compacted bentonite has been specified to perform a range of safety functions for geological waste disposal Wilson et al. (2011). In the Spanish reference concept, as reflected in the FEBEX experiment, the bentonite acts as a buffer between the waste container/heater and the host rock. However, the swelling and sealing characteristics that make it desirable for such an application also make its behaviour complex to predict. The ‘standard’ mechanical and hydraulic models for clays and soils have frequently been shown to be unsuitable for compacted bentonite (e.g. Alonso et al, 1998; Nguyen et al, 2005; Sánchez et al, 2005). Therefore there has been a significant effort in developing and improving thermal-hydro-mechanical (THM) constitutive models for bentonite as part of the FEBEX project, as well as elsewhere in the international radioactive waste management community. This is because the ability to characterise bentonite evolution under repository conditions sufficient to support key safety arguments, as well as inform the general understanding of dynamic bentonite systems, are important elements in building confidence that the overall safety functions required of the bentonite can be relied upon.

Radioactive Waste Management (RWM) has participated in FEBEX-DP through funding the modelling studies reported herein. Participating in FEBEX-DP alongside other
international projects gives RWM the opportunity to continue developing capability in modelling coupled THM processes in bentonite, as well as increasing understanding in the ability of current physical models to predict the evolution of bentonite buffers. The extensive dataset that has been collected over the past ~18 years provides an opportunity to improve physical models and basic understanding of bentonite to extend RWM’s capability in this area.

The work documented here was carried out in two phases:

**Phase 1** applied the Internal Limit Model (ILM, Thatcher et al, 2016), which Quintessa have developed through work with RWM, to FEBEX bentonite for the first time. The aim of this phase was to determine whether the model captured the behaviour of FEBEX bentonite in laboratory and field scale experiments.

**Phase 2** considered improvements to the model equations and modelling assumptions to test whether a better fit of the model to the FEBEX in situ experimental data was possible. In particular, an improved fit of the spatial distribution of dry density and water content within the bentonite was sought.

The ILM is described in Section 2, Phase 1 work is described in Section 3 and Phase 2 work is described in Section 4. The preferred modelling approach, in light of Phase 2 is discussed in Section 4.6 and conclusions from the work in Section 5.

### 1.1 Objectives

In summary, the objectives of this work are:

- To test the ILM approach on FEBEX bentonite;
- To determine whether the ILM is capable of reproducing observations in the FEBEX experiment;
- To investigate whether it is possible to find a single model parameterisation capable of representing bentonite behaviour in a range of experiments; and
- To use the data available in FEBEX to inspire further developments of the ILM.
2 Initial model description

Quintessa developed a hydro-mechanical model of bentonite as part of work for RWM in the DECOVALEX-2015 programme (Bond et al., 2015a). The model was developed to represent an MX-80 bentonite and sand mixture, used in the SEALEX experimental programme at the Tournemire Underground Research Laboratory (URL). During development of the model, a range of representations of the hydro-mechanics were tested and the ILM (Internal Limit Model; Thatcher et al., 2016) was preferred because it explicitly couples the mechanics and hydraulics through relationships derived directly from the data. This is a new model not found previously in the literature, and has been called the Internal Limit Model, as it attempts to describe a fundamental limiting behaviour of the bentonite that links together the hydraulic and mechanical processes (see Section 2.1).

The ILM referred to the system of equations used to represent bentonite: the mechanical processes are based on the Modified Cam Clay (MCC) model; hydraulic processes are based on Richards equation; and thermal processes, which have been added as part of the current work, are based on the diffusion equation. The ILM uses a curve, which we have called the Internal Limit Curve (ILC), to define the water retention function and the shape of the plastic failure surface of the bentonite in addition to explicitly coupling stress and suction.

The model is implemented in Quintessa’s in-house multi-physics code QPAC (Quintessa, 2013).

2.1 The Internal Limit Curve

The ILC (Thatcher et al., 2016) is based on the observation made by a number of authors that, for a given composition of bentonite, one can define a log-linear relationship between the swelling pressure\(^1\) \(P\) and the void ratio \(e\) of the bentonite (e.g. Wang et al., 2012, Bucher et al., 1986). This relationship has the form:

\[
P = P_0 \ast \exp(e\lambda)
\]

Equation 1

where \(P_0\) and \(\lambda\) are constants and \(e\) is the void ratio, which can be expressed in terms of the dry density \((\rho_{dry})\) and grain density \((\rho_{\text{grain}})\) by:

\[
P = P_0 \ast \exp((\rho_{\text{grain}}/\rho_{dry} - 1)\lambda).
\]

Equation 2

\(^1\) Swelling pressure is defined as the pressure reached when bentonite equilibrates with water at atmospheric pressure under constant volume conditions.
Using the swelling experiment data for MX-80 from Wang et al. (2012) as calibration (Figure 2-1), appropriate values for the constants $P_0$ and $\lambda$ can be determined as 745 MPa and -8.5, respectively.

The relationship given by Equation 1 can also be compared against data from oedometer tests (Wang et al., 2013), which were conducted separately from the swelling experiments. In these experiments, the bentonite is loaded, and deforms along a stress pathway, part of which is known as the “virgin consolidation curve”. Figure 2-2 shows Equation 1, with the same parameterisation as used in Figure 2-1, plotted against data from the oedometer tests. Equation 1 fits the part of the oedometer data that represents the virgin consolidation curve.

It has been observed previously (Börgesson et al., 1995) that the virgin consolidation curve and the swelling pressure can be represented by very similar curves. A new feature in the ILM is that Equation 1 is also used to represent the water retention curve for bentonite under free swelling conditions. Assuming the voids are saturated with water, the relationship in Equation 1 between swelling pressure and void ratio can be used to determine a relationship between suction pressure and water content\(^2\) (Figure 2-3). This relationship fits the data when the bentonite is able to swell freely (i.e. there is no confinement) for water content <25%. At higher water contents, or very low dry density, the chemical properties of the bentonite become more important, so an alternative model would be required to describe the behaviour in these regions.

An expression to describe the constant volume water retention curve shown in Figure 2-3 can be derived from the free swelling curve by subtracting stress based on a relationship suggested by Dueck (2005), following from the work of Croney et al. (1958):

$$\Psi = \Psi_{\text{free}} - p$$

Equation 3

where $\Psi$ is suction, $\Psi_{\text{free}}$ is the suction under free swelling conditions and $p$ is the confining stress.

\(^2\) Water content is defined as the ratio of the mass of water to the mass of solid.
Figure 2-1: The ILM curve (Equation 2) fitted to swelling data for MX-80 bentonite with a 70/30 ratio of bentonite and claystone (Wang et al., 2012).

Figure 2-2: Oedometer test data (loading and unloading) (Wang et al. (2013)) for 1.67 Mg/m³ samples of MX-80 bentonite at different suctions (s) with the ILM curve (Equation 1, with \( P = \sigma_v \), \( \sigma_v \) is vertical stress) derived from the Wang et al. (2012) swelling data shown. This curve is a good fit to the part of the data known as the virgin consolidation curve.
The observation that a single “Internal Limit Curve”, of the form given in Equation 1, can be used to fit swelling data, oedometer data and suction data is interesting because it suggests that there could be a fundamental limit within the bentonite that determines the bentonite’s ability to hold both stress and suction. When the stress in the bentonite exceeds the limiting amount of stress, the bentonite will fail plastically. The data indicate that for a fixed mineralogical composition, this limit depends solely on the dry density of the sample. Incorporating these observations results in a model in which the swelling pressure, virgin consolidation curve and suction curve at lower water contents can all be determined from a single set of data, used to calibrate the model’s two parameters. Swelling pressures and suctions in the model will be independent of the path to reaching these states.

Figure 2-3: Water retention data for MX-80 bentonite with the ILM curve (Equation 2 with $\rho_{\text{dry}} = \theta \rho_w/wc$, where $\theta$ is porosity, $\rho_w$ is water density and $wc$ is water content) derived from the Wang et al. (2012) swelling data.
2.2 ILM for FEBEX

The relationships between dry density, stress and suction that were developed for the MX-80 bentonite in the SEALEX experiments (Section 2.1) were tested to check whether they hold for the FEBEX bentonite. As can be seen in Figure 2-4, Figure 2-5 and Figure 2-6, a single ILM curve of the form \( P = P_0 \times \exp(e \lambda) \) (Equation 1) used in the way described in Section 2.1 can be found that fits all three data sets \((P_0 = 1500 \text{ MPa}, \lambda = -7)\). The fit for FEBEX bentonite is not as good as for the SEALEX experiments (Section 2.1). The oedometer data from the FEBEX experiments are only just starting to show plastic deformation at the maximum load, so the ILM curve represents the asymptote that the data are trending towards. This asymptote and the swelling pressure data could be fitted very well by the same curve, but in order to also fit the water retention data, a curve that sits slightly above the swelling pressure and oedometer data was chosen. This could result in overestimation of swelling pressures in the models.

For the FEBEX bentonite, suction is higher than would be predicted based on the swelling and oedometer data using the relationships derived for MX-80 bentonite. This could be due to the differing chemistry of the MX-80 bentonite and the FEBEX bentonite (for example, FEBEX has a higher smectite content than MX-80) which could affect how water is distributed between interlayers and macropores. Alternatively, the suction in the SEALEX experiments could have been affected by mixing bentonite with sand.

Nevertheless, there are clearly relationships between section, swelling and compressive stress in the FEBEX bentonite and ILM curve has the same general form as the data so the approach was used to look at experiments using FEBEX bentonite. To make the ILM curve temperature-dependent, water retention curves at different temperatures (Figure 2-6) were used to determine the following relationship for \( P_0 \):

\[
P_0 = -7.895[\text{MPa.K}^{-1}]T + 1674[\text{MPa}]
\]  

Equation 4

where \( T \) is the temperature (K).
Figure 2-4: Swelling data for the FEBEX bentonite (Lloret et al., 2005) with the calibrated ILM curve.

Figure 2-5: Oedometer test data for the FEBEX bentonite (Lloret et al., 2005) with the calibrated ILM curve.
Figure 2-6: Confined water retention data for the FEBEX bentonite at different dry densities and temperatures (Lloret et al., 2005) compared with the calibrated ILM suction curve for unconfined conditions at 60°C. The departure of the data from the straight line ILM curve represents samples becoming confined and thus stresses building up. The increase in stress reduces the suction in the sample (Equation 2). The ILM curve is used to represent the water retention data where the sample is unconfined; once the sample becomes confined, Equation 2 is used.

2.3 Thermal model

Movement of heat is represented by conduction and convection (coupled to the flow of water vapour) using the equation for heat diffusion with additional fluxes to represent convection. A relationship between saturation ($\phi$) and thermal conductivity ($\lambda_t [W/m/K]$) has been used successfully for many years in the FEBEX experiment (e.g. Rutqvist and Tsang, 2003), so the same relationship was used here:

$$\lambda_t = 1.28 [W/m/K] - \frac{0.71[W/m/K]}{1 + \exp((\phi - 0.65)/0.1)}$$

Equation 5

The specific heat capacity ($c_p^{bulk}$) is calculated as a mass weighted average of the heat capacity of dry bentonite ($c_p^b$) and water ($c_p^w$):

$$c_p^{bulk} = \frac{m_b c_p^b + m_w c_p^w}{m_{total}}$$

Equation 6

where $m_b$ is the dry mass of bentonite, $m_w$ is the mass of water within the sample, and $m_{total}$ is the total mass of the sample.
2.4 Hydraulic model

Water movement in the bentonite is represented by Richards equation; gas is assumed to remain at atmospheric pressure and move freely through the sample, whereas water movement is calculated along pressure and suction gradients under variably saturated conditions.

Porosity ($\theta$) is related to the dry density of the bentonite such that:

$$\theta = 1 - \frac{\rho_{\text{dry}}}{\rho_{\text{grain}}}$$  \hspace{1cm} \text{Equation 7}

Intrinsic permeability ($k$) evolves with porosity following a relationship given in Lloret et al. (2005), derived for FEBEX bentonite, where $k_0$ is a constant (see Section 2.6):

$$k = k_0 \exp(30(\theta - 0.4))$$  \hspace{1cm} \text{Equation 8}

The saturation ($\phi$) dependent relative permeability ($k_{rel}$) is given by:

$$k_{rel} = \phi^3$$  \hspace{1cm} \text{Equation 9}

again, following work on FEBEX bentonite reported in Lloret et al. (2005).

Water pressure ($P_w$) is calculated by subtracting the suction ($\Psi$) from the gas pressure ($P_g$):

$$P_w = P_g - \Psi$$  \hspace{1cm} \text{Equation 10}

Suction under free swelling conditions ($\Psi^{\text{free}}$) is calculated using the ILM curve, using a void ratio ($e^{\text{sat}}$) which is based on the water content, assuming the sample is fully saturated:

$$\Psi^{\text{free}} = P_0 \exp(e^{\text{sat}} \lambda)$$  \hspace{1cm} \text{Equation 11}

For the SEALEX experiment, an additional term was required to represent the behaviour at water content above 30 wt%. This has not been included in the models of the FEBEX bentonite, as the water contents do not reach such a level.

Net suction is related to stress and suction under free swelling conditions through the relationship proposed by Dueck in Equation 3. A new approach taken in this work is to assume that the bentonite grains are orientated in random directions such that a third of the grains are aligned to each principal direction ($i, j, k$). Stress in each of the three principal directions is assumed to act on the third of the grains that are aligned in that direction such that grains aligned in the direction of highest stress will have less capacity to attract water than grains in lower stress directions. This is implemented in the model by introducing a concept of “directional suction” ($\Psi_{nn}$) as:

$$\Psi_{nn} = \Psi_{nn}^{\text{free}} - \sigma_{nn} \text{ for } n = i, j, k$$  \hspace{1cm} \text{Equation 12}

Where stress in each direction is given by $\sigma_{nn}$. The average suction ($\Psi$) given by:
\[ \Psi = \frac{1}{3}(\Psi_{ii} + \Psi_{jj} + \Psi_{kk}) \]  
\text{Equation 13}

The net suction in each of the three directions is constrained such that the average water content over the three directions is equal to the water content calculated from Richard’s equation. More conventional approaches assume that water sits in pores and behaves as a continuous phase, but because water is primarily contained within the bentonite grain structure, this new approach could reflect the physical disposition of water more accurately. However, it should be recognised that representing the water disposition explicitly in this manner is a novel approach and has not yet been widely-adopted in coupled thermal-hydraulic-mechanical modelling.

### 2.5 Mechanical model

The mechanical model is based on the Modified Cam Clay (MCC) model (Roscoe and Burland, 1968). In the MCC, elastic deformation is given by:

\[ v = v_k - \kappa \ln p' \]  
\text{Equation 14}

and the plastic yield surface is given by:

\[ \left[ \frac{q}{k_M} \right]^2 + p'(p' - p_c) = 0 \]  
\text{Equation 15}

whilst the virgin consolidation line has the equation:

\[ v = \Gamma - \lambda \ln p' \]  
\text{Equation 16}

where \( v \) is the specific volume (\( v = 1 + e \), where \( e \) is the void ratio), \( p' \) is effective stress (which equals stress because pore pressure is always less than zero), \( q \) is deviatoric stress, \( p_c \) is the pre-consolidation pressure (which is a point on the virgin consolidation line) and \( v_k, \kappa, M, \Gamma \) and \( \lambda \) are all constant parameters. An associated plastic flow rule is assumed.

Some small modifications were made to the MCC model for the work presented here. The elastic equation in the MCC model gives a linear volume change with the logarithm of effective stress, but the oedometer data in the SEALEX experiment (unloading curve in Figure 2-2) showed a linear trend with stress (rather than log stress) during elastic deformation. Elastic deformation is represented by conservation of momentum with a stiffness matrix dependent on Young’s Modulus and Poisson’s ratio. Poisson’s ratio is a constant and Young’s Modulus is dependent on stress (see Thatcher et al, 2016 for details):

\[ E = \kappa_0 - \kappa_1 p'. \]  
\text{Equation 17}

The plastic yield surface in the models is the same as the MCC yield surface, but the virgin consolidation curve is based on the ILM relationship in Equation 1. The
preconsolidation pressure (which lies on the virgin consolidation line) is given by the ILC:

\[ p_c = P_0 \times \exp(e\lambda) \]  

Equation 18

Swelling of the bentonite is added as a strain source term in the mechanical calculations and is calculated based on the change in water content from initial conditions, calculated by the flow equations. Swelling strain is calculated in the three principal directions such that the volumetric strain is determined by the volume of water added as follows:

\[ \varepsilon_{\text{swell}} = \frac{a}{3} \frac{(\omega_{nn} - \omega_0)m_s}{\rho_w V_{\text{comp}}} \]  

Equation 19

where \( \omega_0 \) is the initial water content, \( \omega_{nn} \) is the water content in direction \( n \), \( m_s \) is the mass of solids, \( \rho_w \) is the density of water, \( V_{\text{comp}} \) is the compartmental (numerical model cell) volume and \( a \) is a swelling efficiency term which reflects that not all additional water will cause a volume increase, some will just fill void space in the sample. The water content in each direction is calculated such that the total amount of water in a compartment is equal to that calculated by the hydraulic model. Water is partitioned into the three directions such that suction, calculated from Equation 11, is equal in the three directions. Free suction in Equation 12 is calculated from Equation 11.

Thermal strains are represented in the model through a linear coefficient of thermal expansion (1x10\(^{-5}\) K\(^{-1}\)) which is applied to the compartment (cell) volumes. This assumes that the thermal expansion of the volume of the compartment is equal to the thermal expansion of the grains and the porosity remains unchanged.

In addition to the MCC plastic failure surface used for failure in compression, a simple failure surface for failure in tension was used. Bentonite is very weak in tension, so the tension failure model assumes that as soon as normal stresses become tensile, plastic failure occurs rapidly in that direction to reduce the tensile stress to approximately zero. Incorporation of tensile failure was required when fitting to the SEALEX experiment to ensure adequate radial expansion of the bentonite samples when resaturated from an outer annulus.

### 2.6 Parameters

The ultimate aim of modelling bentonite systems is to predict their behaviour in the post-closure phase of a geological disposal facility. Developing models that are capable of prediction relies on being able to parameterise the models from prior data for the given bentonite composition and achieve good results without the need for detailed calibration of the model parameters at all relevant scales of interest. The approach to the modelling has therefore been to take the previous physical relationships as developed for the SEALEX experiment (Thatcher et al., 2016), update the parameterisation using data for
FEBEX bentonite and create a single parameter set (Table 2-1) calibrated to all the experimental data. In calibrating to all the experimental data (experiments in Table 3-1 plus the in situ experiment), the fit of the model to each individual experiment may be less good but there is the advantage of finding parameters that are more generally applicable to the FEBEX bentonite. In reality, some further calibration of parameters, particularly permeability, was required for individual experiments, and this is documented in the model description in subsequent sections.
Table 2-1: Parameters used for FEBEX bentonite derived by calibrating to experiments discussed in Section 3. These parameters are used in all models except where stated in Table 3-1.

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<th>Mechanical parameters</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Poisson’s ratio</td>
<td>0.27</td>
<td>Based on Thatcher et al., 2016</td>
<td></td>
</tr>
<tr>
<td>$\kappa_0$</td>
<td>Parameter for elastic deformation, Equation 17</td>
<td>100 MPa</td>
<td>Calibrated to the in situ experiment</td>
</tr>
<tr>
<td>$\kappa_1$</td>
<td>Parameter for elastic deformation, Equation 17</td>
<td>30</td>
<td>Based on Thatcher et al., 2016</td>
</tr>
<tr>
<td>$M$</td>
<td>Gradient of the critical state line.</td>
<td>1.25</td>
<td>Based on Thatcher et al., 2016</td>
</tr>
<tr>
<td>$a$</td>
<td>Swelling efficiency</td>
<td>0.5</td>
<td>Based on Thatcher et al., 2016</td>
</tr>
</tbody>
</table>
3 Phase 1 – Application of the ILM to FEBEX Experiments

3.1 Approach

In Phase 1, a range of FEBEX experiments have been modelled, from laboratory tests to the in situ experiment. The laboratory tests were chosen in particular to test the ILM through varying stages of complexity, and to develop the thermal process model that had not been implemented previously.

Throughout the FEBEX programme there have been a wide range of laboratory experiments performed to characterise the behaviour of the FEBEX bentonite. These laboratory experiments are useful in developing models because they often explore a subset of the coupled processes that occur in the bentonite, for example, oedometer tests at constant suction and constant temperature can be represented by a mechanical model only and constant temperature infiltration tests can be represented by a coupled hydro-mechanical model. Modelling the laboratory experiments therefore provides the opportunity to test parts of the coupled THM model in isolation, which simplifies calibration steps and builds confidence in the process models.

Four laboratory experiments were chosen from the large number available. The experiments were chosen because they tested different processes and couplings as shown in Table 3-1.
Table 3-1: Laboratory experiments modelled

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Processes modelled</th>
<th>Section</th>
<th>Calibrated parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Suction controlled oedometer (Lloret et al, 2005)</td>
<td>M(h)</td>
<td>Section 3.2</td>
<td>$\kappa_0$ 50 MPa</td>
</tr>
<tr>
<td>Constant temperature infiltration with loss of confinement (Lloret et al, 2005)</td>
<td>HM</td>
<td>Section 3.3</td>
<td>permeability $5 \times 10^{-21} \text{ m}^2$</td>
</tr>
<tr>
<td>Infiltration with thermal gradient (Villar et al, 2005)</td>
<td>TH(M)</td>
<td>Section 3.4</td>
<td>permeability $5.8 \times 10^{-21} \text{ m}$ $k = k_0 \theta$</td>
</tr>
<tr>
<td>Heating with no infiltration (discussed in Bond and Watson, 2008)</td>
<td>THM</td>
<td>Section 3.5</td>
<td>None</td>
</tr>
</tbody>
</table>

3.2 Suction controlled oedometer tests

Suction controlled oedometer tests were performed at CIEMAT (Spanish public research centre for energy and environment) on five samples (Section 3.1.1.1 of Lloret et al, 2005). The tests involved taking five samples of bentonite, applying a different suction to each sample and then loading the samples to different stresses. The samples were allowed to equilibrate between each change in boundary conditions. These experimental stages are shown in Table 3-2.

All five samples (S1 – S5) had the same initial vertical stress of 0.1 MPa and very similar suction, around 125 MPa (Path I). Different suctions were then applied to each sample, all under a constant vertical stress (Path II). Where suction was increased (samples S1), the sample contracted and where suction was decreased (samples S3, S4 and S5), the sample expanded. The void ratio of each sample was measured once the sample had reached an equilibrium state. Once the samples had equilibrated, the samples were loaded to either 5 MPa or 9 MPa (Path III). As the samples compressed under the load, the void ratio was measured.
Table 3-2: Stress ($\sigma_v$) and suction ($s$) paths for five samples (Lloret et al, 2005).

<table>
<thead>
<tr>
<th>Test</th>
<th>Initial conditions</th>
<th>Path ($\sigma_v$ (MPa), $s$ (MPa))</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Dry density g/m$^3$</td>
<td>Water content</td>
</tr>
<tr>
<td>S1</td>
<td>1.72</td>
<td>13.0</td>
</tr>
<tr>
<td>S2</td>
<td>1.68</td>
<td>13.7</td>
</tr>
<tr>
<td>S3</td>
<td>1.69</td>
<td>14.2</td>
</tr>
<tr>
<td>S4</td>
<td>1.71</td>
<td>12.9</td>
</tr>
<tr>
<td>S5</td>
<td>1.72</td>
<td>13.2</td>
</tr>
</tbody>
</table>

As the suction is applied to the sample and the data available have no time component, only mechanical processes can be calibrated. In making this simplification, there is the implicit assumption that the sample has a homogeneous water content at the end of each pathway step. In the ILM, the suction is used to calculate the water content and thus the swelling, so it is just fixed at the appropriate values for the experiments.

The parameter values used in the model are as described in Section 2, with the exception of $v_0$. Modelling results were much improved when the value of $v_0$ was reduced from 100 MPa to 50 MPa. This change was made purely on the basis of an improved calibration.

The initial conditions in the model reflect the initial suction and stress given in Path I (Table 3-2). The boundary conditions are zero displacement around the sides and bottom of the sample with a specified stress acting vertically downwards on the sample.

A comparison of stress versus void ratio shows that the modelled results can reproduce the data quite well (Figure 3-1). In particular, the gradients on the loading curves are captured well by the model. The weaker part of the modelled result is the swelling model, which reproduces the volume change well for cases S1 and S5, but less well for cases S3 and S4. From Figure 3-1, it seems clear that some more work is required on the swelling model (although noting that sample heterogeneity may be a factor in the different swelling results), whilst the model of elasto-plastic deformation captures the trends in the data well. In the in situ FEBEX experiment, there is limited void space in
the tunnel, so swelling under low stress, as seen at the start of the oedometer experiments, is not expected to play a large role in the in situ experiment.

![Oedometer test data at different suctions from the CIEMAT experiment with the QPAC model results. Path I to Path II corresponds to movements from the initial suction/void ratio to an imposed suction and subsequent void ratio at a constant vertical stress, thus is represented by vertical lines along the y-axis. Path II to Path III is represented by the increase in vertical stress to the final value for Path III shown in Table 3-2.]

**Figure 3-1:** Oedometer test data at different suctions from the CIEMAT experiment with the QPAC model results. Path I to Path II corresponds to movements from the initial suction/void ratio to an imposed suction and subsequent void ratio at a constant vertical stress, thus is represented by vertical lines along the y-axis. Path II to Path III is represented by the increase in vertical stress to the final value for Path III shown in Table 3-2.

### 3.3 Constant temperature infiltration test with loss of confinement

A new ceramic device was developed by CIMNE (International Centre for Numerical Methods in Engineering, Spain) to carry out infiltration tests under isothermal, controlled temperature gradient and controlled heat flux conditions (Section 3.1.4.2 of Lloret et al, 2005). However only one test was carried out because the device cracked during the first experiment due to the pressure exerted by the bentonite. The experimental data shows a phase where confinement of the bentonite is maintained followed by a phase with no radial confinement. In this test, water was injected into the sample from the top under a hydraulic overpressure of 0.1 MPa. The sample was initially 70 mm in diameter and 140 mm in height, with a dry density of 1.62 g/cm³ and a water content of 13.5%. The test was carried out at isothermal conditions (22°C).
Both hydraulic and mechanical processes are important in this model as the amount of water in the sample will depend on the suction gradient through the sample, and the suction depends on the stresses and void ratio in the sample.

A 2D axis-symmetric model grid is used with vertical discretisation and 2 radial compartments (Figure 3-2). The mechanical model is parameterised as for the oedometer tests, but the permeability had to be calibrated to the data. A calibrated reference saturated permeability of \(5 \times 10^{-21} \, \text{m}^2\) was used instead of \(2.5 \times 10^{-21} \, \text{m}^2\) to obtain a better fit of the model to the data. In the model, the sample was initially under no stress and had an initial water content of 13.5% as in the experiment. The hydraulic boundary conditions in the model imposed a pressure on the top surface of 0.1 MPa above atmospheric pressure. The mechanical boundary conditions enforce zero displacement on all external surfaces until day 7, when radial confinement was lost. Thereafter a stress of 0.1 MPa was applied radially.

![Figure 3-2: Grid showing discretisation and coloured according to z-value.](image)

Comparing the vertical stress in the model to that measured in the experiment shows that the model does not capture the vertical stress well (i.e. swelling pressure Figure 3-3), although the amount of water entering the model is approximately correct (Figure 3-4). The parameterisation of the mechanical processes is exactly the same as in the oedometer tests, where swelling was in some cases underestimated. However, Figure 2-4 indicates that we might expect the models to overestimate swelling pressure, so the model is consistent with the parameterisation. Again, this points towards the need for further work on the swelling model for a pure compacted bentonite rather than the bentonite/sand mixture used in the SEALEX experiment. The amount of water injected into the sample is approximately correct, although the modelled injection rate is too slow at the start and end (Figure 3-4). This level of fit between the model and data was deemed to be sufficient for the purpose of constraining the hydraulic model for the in situ test,
and is consistent with fits obtained in other bentonite modelling activities for water intake (Lloret et al, 2005).

Figure 3-3: Swelling pressure developed during the infiltration test (Lloret et al, 2005) compared with the modelled pressure response from QPAC.

Figure 3-4: Volume of water injected prior to the loss of containment (Lloret et al, 2005) compared with the modelled volumes from QPAC.
3.4 Infiltration with thermal gradient

Infiltration experiments were performed at CIEMAT in steel cells with an internal diameter of 7 cm and an inner length of 40 cm, as shown in Figure 3-5 (Villar et al, 2005). Experiments were performed both at a constant temperature and under a thermal gradient. Both cases have been modelled here with relative humidity and water inflow compared with measurements.

In the isothermal case, a water pressure of 1.2 MPa was applied at the top of the cylinder, and no source of heat was applied.

In the thermal gradient case, a fixed temperature of 100°C was applied at the base of the sample and ambient thermal conditions were maintained at the top of the sample. An insulating jacket, 15 mm thick and with a thermal conductivity of 0.04 W/m/K, was attached around the edge of the cylinder. Hydration started 65 hours after heating with a water pressure of 1.2 MPa at the top of the cylinder.

Temperature and relative humidity in the bentonite were measured at 10 cm, 20 cm and 30 cm from the base of the experiment and the mass of injected water was recorded. There were no measurements of stress.

The model needs to represent thermal and hydraulic processes. Since mechanics and hydraulics are coupled through the suction relationship, mechanical processes also need to be represented, but there are no data from the experiments to help constrain the mechanical model, so more attention was paid to the hydraulic and thermal processes.

The infiltration experiment is represented in the model by a 2D-axisymmetric grid with discretisation in the z-direction and 2 compartments in the r-direction. The parameterisation is as described in Section 2, but to fit the data well an intrinsic saturated permeability of $5.8 \times 10^{-21}$ m$^2$ rather than $2.5 \times 10^{-21}$ m$^2$ was used and the relationship between permeability and porosity was given by $k = k_0 \theta$.

The initial conditions are dry density of 1.655 g/cm$^3$ and initial water content of 13.7%, with initial temperature of 25°C and no stress in the sample.

For the isothermal case, the boundary conditions are zero displacement on all boundaries, with a no flow boundary on the bottom of the sample and a constant pressure boundary of 1.2 MPa on the top boundary after an initial equilibration period of 18 hours at room temperature and ambient humidity, consistent with the experimental set-up.

The case with a thermal gradient has the same boundary conditions, with an equilibration period of 65 hours and additional boundary conditions for the thermal problem. At the top boundary, a constant temperature of 25°C is imposed. Along the side boundaries, a heat flux is calculated based on the temperature gradient across the
thermal insulation, following the method used by Bond and Watson (2008). A fixed temperature of 100°C is specified on the bottom boundary.

The results for the isothermal case show that the general trends of the relative humidity data have been captured by the model, although some of the detail is not, for example, the relative humidity in sensor 3 rises too rapidly (Figure 3-6). There is clearly some scope for further calibration here, particularly of the relationship between permeability, strain and water content. The model does not reproduce the data for the water content injected (Figure 3-7) with the volumes in the model a factor of 2.5 too small, but do have a similar shape to the data. The mismatch between modelled and measured results was found in previous modelling work and is discussed there (Bond and Watson, 2008). There is some question as to whether the data are fully reliable. Indeed, if the data are correct, it would suggest that the sample was significantly over-saturated at the end of the experiment; hence a water leak is strongly suspected.
Figure 3-5: Schematic diagram of the infiltration experiment performed by CIEMAT (Bond and Watson, 2008).
Figure 3-6: Relative humidity during the isothermal infiltration test (Bond and Watson, 2008, after Villar et al., 2005) at locations shown in Figure 3-5 compared with the modelled relative humidity response from QPAC.

Figure 3-7: Volume of water injected during the isothermal infiltration test (Bond and Watson, 2008, after Villar et al., 2005) compared with the modelled volumes from QPAC.
In the test with thermal gradient, there was no infiltration for the first 60 hours whilst the sample was heated. The model results from this period show a reasonable match to the data, with the timing of temperature increase captured well, but the steady-state temperature is slightly underestimated at sensors 1 and 2 (Figure 3-8). The increase in temperature causes an increase in relative humidity, which again, the model slightly underestimates at sensors 1 and 2 due to the temperature underestimate (Figure 3-9).

In the period after 60 hours, there is both heating and infiltration. During this period, diurnal changes in the ambient temperature significantly affect the temperature signal in the experiment, but these ambient temperature changes were not included in the model. The model fits the average temperature well at sensor 3, but again slightly underestimates the temperature in sensors 1 and 2 (Figure 3-10). The model captures all the processes affecting relative humidity, but the response of the model is initially slower than in the experiment (Figure 3-11). At later times, the model seems to diverge from the data, however longer time series shown in Bond and Watson (2008) reveal that the experiment has not reached a steady state relative humidity at 10,000 hours. This is likely to do with permeability estimates, as in the isothermal case, and possibly the vapour diffusivity formulation. A more sophisticated model of vapour diffusivity, which would tend to increase vapour diffusivity overall, especially under thermal gradients (Philip and deVries, 1959), would enhance the drying behaviour and would be straight-forward to implement in a future QPAC model.

Figure 3-8: Temperature change during the first 60 hours of the infiltration test with a thermal gradient (Bond and Watson, 2008, after Villar et al., 2005) at locations shown in Figure 3-5, compared with the modelled temperature from QPAC.
Figure 3-9: Relative humidity change during the first 60 hours of the infiltration test with a thermal gradient (Bond and Watson, 2008, after Villar et al., 2005) at locations shown in Figure 3-5, compared with the modelled relative humidity from QPAC.

Figure 3-10: Temperature change during the infiltration test with a thermal gradient (Bond and Watson, 2008, after Villar et al., 2005) at locations shown in Figure 3-5, compared with the modelled temperature from QPAC.
Figure 3-11: Relative humidity change during the infiltration test with a thermal gradient (Bond and Watson, 2008, after Villar et al., 2005) at locations shown in Figure 3-5, compared with the modelled relative humidity from QPAC.

3.5 Heating test with no infiltration

A heating test with no infiltration was conducted at UPC (Univeritat Politècnica de Catalunya, UPC, 2007) and was used in the THERESA project as a benchmarking test (Bond and Watson, 2008). The experiment involved heating two cylindrical samples of FEBEX bentonite at one end with a fixed temperature on the other end. The samples were arranged symmetrically about the heater, as shown in Figure 3-12, and the experiment was undertaken in a vertical orientation (i.e. rotated 90° compared with Figure 3-12). The samples were surrounded with a latex membrane which does not allow any fluid flow across it but does allow deformation of the sample. The sample was also covered in a layer of thermal insulation which had an estimated thermal conductivity of 0.039 W/m/K and a thickness of 55 mm. The temperature in the bentonite was measured throughout the test and on dismantling, after 7 days of the experiment, the water content and diameter of the samples were measured.
Modelling this experiment requires a full THM representation of the processes. The heating will cause drying close to the heater and vapour will flow away from the heater. A gradient in water content is expected with distance from the heater. This will also affect the mechanical properties of the bentonite, since the wetter bentonite is likely to swell and the drier bentonite to contract. As the experiment is symmetrical, just one cylinder of bentonite was represented in the model.

In addition to the THM model of the bentonite, a thermal model of half of the heater was also included in the model and fully coupled to the THM model of the bentonite. Half of the heating power was applied. Testing of the models showed that including the heater in the model is important as the thermal insulation is not perfect and therefore the heater loses heat radially as well as into the bentonite.

The bentonite model is a 2D axi-symmetric model with discretisation in the z-direction and with 2 compartments in the r-direction. The insulation was accounted for in the boundary condition. The parameterisation is as given in Section 2. The heater is represented as a single compartment.

The initial conditions of the model reflect the initial conditions in the experiment: the bentonite has a dry density of 1.63 g/cm³ and a water content of 15.33%. The initial temperature of the bentonite was 22°C and the bentonite was at atmospheric pressure.

The thermal boundaries on the model consist of a constant temperature of 30°C on the cool end of the bentonite and a heat flux around the outside of the bentonite and heater calculated based on the given thermal conductivity of the insulation and assuming that the outside of the insulation is at ambient temperature. Heat is input into the model as a source term in the heater compartment, at a power of 109 W (only half of the experiment is modelled), but the heat input was also scaled by a factor of 0.8 to calibrate the model (Bond and Watson, 2008). It is not uncommon in heater tests to suspect that the heater is supplying a fraction of the quoted power. The hydraulic boundary conditions are all no flow since the experiment is wrapped in a membrane to prevent fluid loss. The sample
is allowed to deform under atmospheric pressure conditions both lengthways and radially, but with no deformation occurring at the heater.

The comparison between the data and model results shows that the model is able to represent the thermal behaviour of the experiment well (Figure 3-13). The model also does a good job of representing the trend of the water content and diameter increment data (Figure 3-14 and Figure 3-15), although the diameter increment is underestimated at a distance of 70 mm from the heater whilst the water content is captured correctly. This again suggests work is needed on the swelling model.

Figure 3-13: Temperature change during the heating test (Bond and Watson, 2008) at different distances from the heater, compared with the modelled temperature from QPAC.
Figure 3-14: Water content with distance from the heater after 7 days of heating (Bond and Watson, 2008) compared with the modelled water content from QPAC.

Figure 3-15: Diameter increment with distance from the heater after 7 days of heating (Bond and Watson, 2008) compared with the modelled diameter increment from QPAC.
3.6 FEBEX In situ experiment

The geometry of the in situ experiment is shown in Figure 3-16. In 2002 it was decided to turn Heater 1 off and excavate Heater 1 from the experiment. The experiment continued from 2002 until 2015 with only one heater and a dummy heater to fill the hole where Heater 1 had previously been.

The bentonite blocks were emplaced in the experiment at a dry density of 1.7 Mg/m³ such that once swelling had occurred into any void spaces between and around the blocks, the average dry density of the bentonite after emplacement was expected to be 1.6 Mg/m³.

The two heaters were initially switched on at a constant power, but after 61 days they were switched to temperature control whereby the hottest point measured should not exceed 100°C.

Figure 3-16: Schematic diagram of the FEBEX in situ experiment, before and after the removal of Heater 1 (Lanyon and Gaus, 2013).

Several hundred sensors were installed in the experiment to measure temperature, pressure, water content and displacements. In the tunnel most of the sensors were located in vertical sections, as shown in Figure 3-17. There were different sensors in each section, and whilst there are good temperature data throughout the lifetime of the experiment, the majority of the relative humidity sensors reached relative humidity greater than 95% and stopped recording.

An example of the data available in Section F2 is shown in Figure 3-18. The exact radial locations of the sensors are not clear from this figure, but for comparison with the models, the red data points for temperature are assumed to be on the inner surface of
the bentonite next to the heater, red data points for pressure and relative humidity are assumed to be in the first 20 cm of bentonite from the heater and the green data points are assumed to be at the mid-point between the heater and the tunnel wall.

Phase 1 modelling of the in situ experiment starts with the assumption that the experiment can be represented by a 1D model, as the main gradients in temperature and pressure are expected to be in the radial direction. There is some variation in temperature along the heater, so once the 1D model had been built and calibrated, a 2D model was built to capture the longitudinal temperature variation. These two models were included along with models of the laboratory tests in the calibration that was used to determine the parameters in Section 2.6. Phase 2 modelling (Section 4) builds on the Phase 1 model by considering whether any updated process models could improve the fit of the model to the data.
Figure 3-18: Data and locations of instruments from the in situ test for Section F2, which is positioned at the centre of Heater 2. Dashed vertical lines shows changes in boundary conditions including switching off and removal of Heater 1 (Lanyon and Gaus, 2013).
3.6.1 1D In situ experiment model

The data from the in situ experiment show axial symmetry, so as a first approximation, a 1D model was developed of the bentonite extending from the heater surface to the tunnel wall (Figure 3-19). A fully coupled thermo-hydro-mechanical model was used to represent a section of bentonite positioned at the centre of the heater.

![Figure 3-19: Model grid used in the 1D in situ test model, coloured according to radial distance.](image)

The model is parameterised as in Section 2.

The temperature in the granite host rock and in the gallery is 12°C, so the initial temperature in the bentonite is specified as 12°C in the model. The initial water content of the bentonite is 14.4% and the dry density is 1.6 g/cm³. We are not explicitly modelling any gaps between bentonite blocks, so the initial dry density reflects the average dry density expected once the bentonite has swelled into all the void space. There is no initial stress in the bentonite.

The thermal boundary condition on the inside of the bentonite represents the heater in the experiment. The detail of the initial heating has not been included in the model, and instead a constant temperature is prescribed on the inside surface of the model. The model represents the central part of the heater (Section F2), which is the hottest part of the heater. The temperature measurements from this part of the heater show that at the base of the heater the temperature is 100°C, but at the side the temperature varies between 93°C and 95°C. There are data obtained at early times from the top of the heater, which look similar to the side of the heater, so the fixed temperature at the heater has been set to 94°C in the model to simulate the upper half of the heater.

The outer boundary has a fixed heat flux calculated assuming ambient temperature at 2 m into the granite, designed to approximate the heat flux out of the bentonite, rather than accurately reproduce the temperature in the granite.
The hydraulic boundary conditions are no-flow apart from the bentonite-tunnel wall surface where water may flow into the bentonite from the rock. Prior to installation of the FEBEX experiment, water was flowing into the FEBEX drift at a rate of 7.8 mL/min, approximately half of which came from six identified inflow points (Lanyon and Gaus, 2013). The permeability of the granite matrix is generally higher than that of saturated bentonite, so water is expected to move from the granite into the bentonite. To represent this heterogeneous inflow of water in a simplified way, a constant pressure boundary was applied to the model with water at atmospheric pressure. This approximation accounts for the observation that there was little desaturation in the granite due to construction of the tunnel (Lanyon and Gaus, 2013), but may underestimate the hydraulic gradient between the granite and the bentonite, as the water pressure in the granite may be closer to hydrostatic pressure than atmospheric pressure. Since the main hydraulic gradients will be caused by very high suction in the bentonite (initial suction 119 MPa), the precise boundary conditions are not expected to have a significant effect on the resaturation of the bentonite.

The mechanical boundary conditions are zero displacement everywhere.

Modelling results are compared to data from Figure 3-18.

Modelled temperatures are reported on the inner boundary at the heater surface, where the temperature is fixed to be 94°C and at a radial distance half way through the bentonite. The temperature boundary condition matches the data well (Figure 3-20). The values half way through the bentonite also match the data well.

Total pressure measurements are reported on the tunnel wall. The measurements show a delay between the onset of the experiment and the build-up of pressure at the tunnel wall due to the time taken for swelling into the void space between the bentonite blocks and the tunnel wall (Figure 3-21). The difference in pressure between the base of the tunnel (location 1) and the other three measurement locations is likely to be due to different densities of bentonite caused by swelling into void space, with less void space beneath the heater and therefore higher net bentonite density. There is no information on the void space in the tunnel at the start of the experiment, so this has not been represented. The model results are reported close to the tunnel walls but just inside the bentonite. Since there are no voids in the model, pressure rises immediately at the start of the experiment and does not show the delay seen in the data. The rate of pressure increase is also faster in the model than in the data and this is likely to be related to the fast increase in relative humidity in the model. The model and experiment are consistent in the asymptotes that the pressures are trending towards.

Relative humidity measurements and model results are from the same locations, in the middle of the bentonite and close to the tunnel wall. At the tunnel wall, the agreement between model and data is very good, with the model sitting in between the two measurement series (Figure 3-22). In the middle of the bentonite the fit is good, although
the modelled humidity rises much more quickly than the data. This could be related to a lack of ‘gap’ to be swollen into, and hence stress building up more rapidly in the model (which will tend to increase the relative humidity) than in the experiment, alternatively, it could indicate that the hydraulic model is allowing too much water to flow into the middle of the bentonite.

As the experiment was dismantled, measurements of water content and dry density with radial distance from the heater were made. These measurements were taken during dismantling of both Heater 1 and Heater 2. The data plotted here are for Heater 1, but the data for Heater 2 are very similar, showing that the redistribution of water and mass happened mostly within the first 5 years of the experiment. The modelled dry density is better close to the container, but has underestimated the change in dry density with distance from the heater (Figure 3-23), again suggesting that explicit modelling of the outer void around the bentonite (as was done for the SEALEX experiment) may lead to better mechanical results. The modelled water content has the appropriate gradient through the bentonite and is at the lower end of the measured values, but fits the data quite well (Figure 3-24). In general, the model underestimates water content but overestimates relative humidity, which suggests the water retention curve requires calibration.

Figure 3-20: Temperature in the in situ experiment (Lanyon and Gaus, 2013) at locations shown in Figure 3-18, compared with the modelled temperature from QPAC (the red QPAC line should be compared to data from locations 2 and 6, which are both close to the heater surface; the green line with data from location 5).
Figure 3-21: Pressure in the rock wall of the in situ experiment (Lanyon and Gaus, 2013) at locations shown in Figure 3-18, compared with the modelled pressure from the outer portion of bentonite.

Figure 3-22: Relative humidity in the in situ experiment (Lanyon and Gaus, 2013) at locations shown in Figure 3-18, compared with the modelled relative humidity from QPAC.
Figure 3-23: Dry density in the in situ experiment (Lanyon and Gaus, 2013) at the central section of Heater 1 after 5 years, compared with the modelled dry density from QPAC.

Figure 3-24: Water content in the in situ experiment (Lanyon and Gaus, 2013) at the central section of Heater 1 after 5 years, compared with the modelled water content from QPAC.
3.6.2 2D In situ experiment model

The data from the experiment show that generally the system has axial symmetry. There are some deviations from this, for example, the heater is hotter at the base than at the sides and top, but in general axial symmetry can be assumed. There is more significant variation along the length of the heater, with the heater surface at the mid-length of the heater between 90°C and 100°C compared to the heater surface at the ends of the heaters being around 80°C. Therefore a 2D model has been built assuming axial symmetry but with heat output from the heater varying along the length of the heater.

The model represents the THM behaviour of the bentonite within the in situ experiment, but does not include the host rock or the plug. It was decided to keep the model as simple as possible to start with, representing only the bentonite as shown in Figure 3-25, and add extra complexity in the form of more geometry at a later stage if necessary.

As for the 1D model, the temperature in the granite host rock and in the gallery is 12°C, so the initial temperature in the bentonite is specified as 12°C in the model. The initial water content of the bentonite is 14.4% and the dry density is 1.6 g/cm³. We are not explicitly modelling any gaps between bentonite blocks, so the initial dry density reflects the average dry density expected once the bentonite has swelled into all the void space. There is no initial stress in the bentonite.

The thermal boundary for the heater is a specified flux boundary, where the flux is constrained such that the hottest temperature on the inside surface (interface) of the heater is 100°C, reflecting how the heater power is determined in the experiment.

The outer thermal boundaries are all mixed boundaries, representing heat fluxes calculated such that the temperature 2 m from the tunnel wall is at ambient conditions, as in the 1D model. These boundaries were calibrated to achieve a sensible temperature distribution through the bentonite. In future modelling, the granite should be explicitly represented to improve the representation of heat flow.

The hydraulic boundary at the heater surface and the two ends of the model are no flow boundaries. Whilst there is inflow from the granite at the end of the tunnel, it is not clear how much water would be flowing into the model here. Since we are mainly interested in matching experimental data at the centre of Heater 2, the boundary is considered to be at a great enough distance to not have any significant effect on the model results of interest. The hydraulic boundary around the outside of the bentonite cylinder is a constant pressure boundary with a water pressure equal to atmospheric pressure as discussed in Section 3.6.1.
Figure 3-25: R-Z section of the model grid for the 2D representation (no angular variation) of the in situ experiment, coloured by temperature at 10 years. Large red compartments in the centre represent bentonite next to the heater – the volume of the heater is not included in the model grid.

The modelled temperature distribution agrees well with the data (Figure 3-26). Over the first five years, there was also heat from Heater 1 in the experiment, so data points close to Heater 1 show some effect of Heater 1, which is not captured in the model (e.g. the early part of Section I). The distribution of temperature at the heater surface (or equivalent radius) shows a good match between model and data (Figure 3-26), indicating that the temperature boundary condition imposed represents the experiment well and that the thermal conductivity in the model is sensible. The radial distribution of temperature (Error! Reference source not found.) is also represented well in the model. Some fine adjustments (e.g. to boundary conditions or thermal properties) may help to improve the fit, but the differences could also be owing to discrepancies between the location of the sensor in the middle of the bentonite and the location of the model output.

The measured relative humidity and modelled values are in reasonably close agreement. In general, the modelled relative humidity increases more slowly than in the experiment (Figure 3-28 and Figure 3-29). This is consistent with previous comparisons between modelled and measured relative humidity (e.g. Figure 3-11). In the longer term, relative humidity at section F2 decreases gradually. This reflects an ongoing slow increase in dry density at this location which relates to suction through the ILC.

The distribution of dry density and water content with radial distance through the bentonite is less similar to the data in the 2D model (Figure 3-30, Figure 3-31) than in the 1D model, but both the 1D and 2D models are similar in having dry density profiles that are flatter than the observed profiles.
Figure 3-26: Comparison of modelled temperature and temperature data from the in situ experiment (data supplied as part of FEBEX project) at a radial distance corresponding to the surface of the heater for sections of the experiment shown in Figure 3-17.

Figure 3-27: Comparison of modelled temperature and temperature data from the in situ experiment (data supplied as part of FEBEX project) at different radial distances in section D2 shown in Figure 3-17.
Figure 3-28: Comparison of modelled relative humidity and relative humidity data from the in situ experiment (data supplied as part of FEBEX project) at a radial distance corresponding to the mid-point between the heater surface and tunnel wall for sections of the experiment shown in Figure 3-17.

Figure 3-29: Comparison of modelled relative humidity and relative humidity data from the in situ experiment (data supplied as part of FEBEX project) at different radial distances in section H shown in Figure 3-17.
Figure 3-30: Dry density in the in situ experiment (Lanyon and Gaus, 2013) at the central section of Heater 1, compared with the modelled dry density from the 2D QPAC model.

Figure 3-31: Water content in the in situ experiment (Lanyon and Gaus, 2013) at the central section of Heater 1, compared with the modelled water content from the 2D QPAC model.
3.7 Phase 1 Conclusions

The aim of Phase 1 was to establish whether the proposed ILM approach is viable for the FEBEX bentonite and to build a model of the in situ FEBEX experiment. These aims have been fulfilled; the basic ILM works for the FEBEX field and laboratory experiments. The previous work on the SEALEX experiment did not include a thermal model, so this has been newly added and coupled to the hydraulic and mechanical models. Thermal data are well represented by the model.

To build confidence in the predictive power of the models, calibration of the models to the data in individual experiments has been kept to a minimum, favouring an approach in which consistent parameter sets were used across a range of experiments, at the cost of possibly producing less detailed fits to the data than could be achieved by detailed calibration. To a large extent, this has been achieved, although there are some notable exceptions, including the parameterisation of permeability for different experiments. This indicates that there is still some work required to produce models that are capable of reliable prediction without the need for significant calibration, but the work documented here is a significant step forward over modelling attempts with new parameter sets for each experiment modelled.

Some consistent disagreements between the model and the experimental data have been noted across different experiments in Phase 1, and were the focus of further work in Phase 2. A number of cases showed the model over-predicting swelling pressures (e.g. constant temperature infiltration with loss of confinement and the 1D in situ model) and under-predicting volume of swelling (laboratory oedometer tests and the dry density distribution for the 1D in situ model). Two possible reasons for these observations are that the ILM curves require an alternative calibration and the swelling model needs further refinement. Furthermore, including the experimental voids in the models may also improve the stress response and dry density distribution.

Comparison of the 1D and 2D model results showed that the 1D-axisymmetric model is sufficient for representing the system at the centre of Heater 2 and therefore the calibration work in Phase 2 will focus on the 1D model, which is easier to change and quicker to run.
4 Phase 2 - Calibrating the in situ model

4.1 Approach

The aim of Phase 2 was to investigate whether any updates can be made to the ILM that will improve the fit of modelling results to the in situ test. The focus was on updating process models which could lead to an improvement in the generalised ILM for any bentonite experiment, rather than calibrating parameters to improve the model fit just for the FEBEX in situ experiment.

From Phase 1, it is clear that swelling pressure is overestimated in the model. This is consistent with the ILM curve chosen for Phase 1, which is a best fit for the water retention data as well as the swelling data and the oedometer data. Fitting all three data sets with one curve resulted in overestimating swelling pressures at a given dry density (Figure 2-4). Alternative calibrations of the ILM curve for the FEBEX data were considered in Phase 2 to reduce the swelling pressure.

A number of teams working on the FEBEX-DP project found it difficult to produce the correct dry density distribution with radial distance from the heater. To address this difficulty, a development of the Barcelona Basic Model (BBM), referred to as the Barcelona Expansive Model (BExM, Alonso et al. 1999) has been used. Using the BExM, teams successfully reproduced the observed dry density gradient. The BExM introduces the concept of two scales of structure within the bentonite: a microstructure in which swelling takes place and a macrostructure in which grain rearrangement occurs. The ILM (see Section 2) offers a simpler approach to modelling THM processes in bentonite than the BBM, and therefore investigations in Phase 2 considered whether there is an equivalent update to the ILM that could improve the dry density distribution given by the ILM.

Work in Phase 2 considered whether an improved dry density profile could be obtained by explicitly including the void between the bentonite and the granite in the model. In addition, numerical experiments were carried out to test whether any alternative formulations of the ILM affect the dry density profile. In previous work on bentonite in cylindrical geometries (e.g. Bond et al 2015b), radial swelling of bentonite into a void space led to elastic expansion of the whole bentonite sample to fill the void, rather than swelling of a small part of the bentonite. This effect was investigated in Phase 2, to see if it is important for the radial distribution of dry density.

Finally, the amount of swelling was identified as a potential area for improvement both in Phase 1 and in previous work (Bond et al., 2015b), and so alternative swelling models were considered in Phase 2.
In Phase 1, the differences between the 1D and 2D representations of the experiment were shown to be small compared to the differences between the models and the data. Since the 1D model is less computationally expensive, work in Phase 2 was carried out on the 1D model to maximise the number of model runs that could be undertaken, and therefore maximise the amount of testing of different ideas. Results below are presented for four models that represent the significant findings from Phase 2.

4.2 ILM calibration

The data for an MX-80 bentonite from the SEALEX experiment showed a very close relationship between the water retention curve and the swelling / plastic failure curve (Section 2.1). Data from the FEBEX bentonite show a less close relationship between the water retention curve and the swelling / plastic failure curve (Section 2.2). Since the two bentonites have significantly different chemical composition, and the MX-80 bentonite was mixed with sand, whereas the FEBEX bentonite was not, it is to be expected that physical relationships that were true in one material are different in another, albeit related, material.

In order to better fit the FEBEX data, the ILM curve was fitted to the swelling and oedometer data and a separate parameterisation was used for the water retention curve. The ILM curve has the form \( P = P_0 \exp(e\lambda) \) and the same value of \( \lambda \) was used for both parameterisations, whilst the values of \( P_0 \) differed by a factor of 2 (Table 4-1). The newly calibrated ILM curves are plotted against the corresponding FEBEX data in Figure 4-1, Figure 4-2 and Figure 4-3 and show a good fit.

Selected results for the in situ experiments from the model with updated ILM parameters are shown in Figure 4-4 to Figure 4-8. The temperature and relative humidity are very similar to Figure 3-20 and Figure 3-22. However, the swelling pressure curve Figure 4-6 is significantly lower than in Figure 3-21, which is consistent with the ILM curve now predicting lower swelling pressures for a given dry density. The radial distribution of dry density Figure 4-7 is slightly flatter than in the previous model (Figure 3-23) and therefore a slightly worse fit, but the water content (Figure 4-8) fits the data considerably better than the previous model (Figure 3-24). Overall, this change resulted in an improved fit of the model to the data from the FEBEX experiment and was more consistent with the material property data (swelling and suction curves) so this new calibration was used in the subsequent models in this report. This calibration has resulted in an additional parameter in the model, and whilst it would be preferable to reduce the number of parameters, the data we have suggest that this parameter is required.
Table 4-1: Parameters for two ILM curves.

<table>
<thead>
<tr>
<th>ILM parameter</th>
<th>Swelling / failure</th>
<th>Water retention</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_0$ [MPa]</td>
<td>650</td>
<td>1300</td>
</tr>
<tr>
<td>$\lambda$ [-]</td>
<td>-6.8</td>
<td>-6.8</td>
</tr>
</tbody>
</table>

Figure 4-1: Swelling data for the FEBEX bentonite (Lloret et al., 2005) with the newly calibrated ILM curve.
Figure 4-2: Oedometer test data for the FEBEX bentonite (Lloret et al., 2005) with the newly calibrated ILM curve.

Figure 4-3: Confined water retention data for the FEBEX bentonite at different dry densities and temperatures (Lloret et al., 2005, additional PT 2002-04 data from Villar, 2002) compared with the newly calibrated ILM suction curve for unconfined conditions at 60°C. For a more detailed discussion of this Figure see Figure 2-6.
Figure 4-4: Temperature in the in situ experiment (Lanyon and Gaus, 2013) at locations shown in Figure 3-18, compared with the modelled temperature from QPAC, using the updated ILM curves (the red QPAC line should be compared to data from locations 2 and 6, which are both close to the heater surface; the green line with data from location 5).

Figure 4-5: Relative humidity in the in situ experiment (Lanyon and Gaus, 2013) at locations shown in Figure 3-18, compared with the modelled relative humidity from QPAC using the updated ILM curves.
Figure 4-6: Pressure in the rock wall of the in situ experiment (Lanyon and Gaus, 2013) at locations shown in Figure 3-18, compared with the modelled pressure from the outer portion of bentonite, using updated ILM curves.

Figure 4-7: Dry density in the in situ experiment (Lanyon and Gaus, 2013) at the central section of Heater 1, compared with the modelled dry density from the QPAC model with updated ILM curves.
Figure 4-8: Water content in the in situ experiment after 5 and 18 years (Lanyon and Gaus, 2013) at the central section of Heater 1, compared with the modelled water content from the QPAC model with updated ILM curves.
4.3 Inclusion of voids

The FEBEX bentonite was installed inside the experiment in blocks, and there were likely to have been small gaps between some of the bentonite blocks, and a larger gap between the blocks and the tunnel wall at the sides and top of the tunnel. This could affect the dry density and water content distributions in the bentonite. Since the gap between the tunnel and the bentonite is thought to have been the largest gap in the system, due to the practicalities of installing the bentonite, this gap was explicitly represented in the model.

The gap is represented by a boundary condition that allows free swelling until a displacement threshold, which corresponds to the width of the gap, is reached. After this point, the boundary is very stiff such that further swelling is almost completely inhibited. In conjunction with this boundary condition, the initial dry density of the bentonite was updated to reflect the true installed dry density of the bentonite blocks. In comparison, the previous model used the net dry density including all the voids in the tunnel.

The model results are improved in that they show a slower increase in swelling pressure since stress in the radial direction only builds up once the radial void is closed (Figure 4-9 compared with Figure 4-6). Otherwise, the results are not changed significantly with the addition of a void. The void was retained for subsequent models.
Figure 4-9: Pressure in the rock wall of the in situ experiment (Lanyon and Gaus, 2013) at locations shown in Figure 3-18, compared with the modelled pressure from the outer portion of bentonite, using updated ILM curves and including a void space.
4.4 Alternative implementation of deformation in a cylindrical geometry

The FEBEX experiment, with a heat source on the inner annulus and a water source on the outer annulus, has a cylindrical geometry. The equations that describe elastic deformation in cylinders include a strong link between radial and angular deformation; as the radius increases, so too must the circumference of the cylinder to ensure continuity of the solid. This is not the case in a Cartesian geometry where it is possible to have deformation in only one coordinate direction.

For the FEBEX in situ experiment, a consequence of the link between stresses in the radial and angular direction is that, when the outer part of a cylinder expands due to swelling, bentonite closer to the axis of the cylindrical model also expands in both the radial and angular direction (Figure 4-10, top conceptual model). This expansion without the corresponding swelling and/or thermal expansion in the inner parts of the cylinder places the bentonite into tension. The ILM includes a simple tensile failure criterion which prevents significant tensile stresses from being developed (most soils are very weak in tension), but this alone is not enough to generate the large degree of density variation seen in the in situ experiment.

Other modelling teams had difficulties in representing the density gradient through the bentonite, and most teams who resolved this adopted the Barcelona Expansive Model (BExM). To remain consistent with the approach of looking for simpler solutions than the BBM / BExM, an alternative representation of the bentonite was sought which could reproduce the observations.

An alternative conceptual model for bentonite is that the addition of water to the outer circumference of a cylinder will cause the outer portion to swell, but this will not create tensile stress or other body forces that cause the inner parts of the cylinder to also expand (Figure 4-10, bottom conceptual model). This would help to explain the steep gradient in dry density observed in the experiment. However, this behaviour is not consistent with standard theory for linearly elastic materials. Experiments were performed with the ILM to try and reproduce this conceptual behaviour, by testing different conceptual models and numerical implementations, one of which was able to reproduce the conceptual behaviour.

The equations that are used to relate stress and strain in linear elastic materials are given in Appendix A for both cylindrical and Cartesian geometries. The general equation that is solved is Newton’s second law:

\[ \rho \frac{\partial^2 \bar{u}}{\partial t^2} = \nabla \bar{\sigma} - \bar{B} \]

Equation 20
where $\rho$ is density (kg/m$^3$), $u$ is displacement (m), $t$ is time (s), $\sigma$ is stress (MPa) and $B$ are body forces (N/m$^3$). In a Cartesian geometry, the body forces are equal to zero unless the body is subject to external acceleration (e.g. gravitational acceleration, rotation, etc.). For example, the acceleration due to gravity when included in the $\bar{B}$ term is:

$$\bar{B} = \begin{pmatrix} \rho g_x \\ \rho g_y \\ \rho g_z \end{pmatrix}$$ \hspace{1cm} \text{Equation 21}$$

Where $g_x, g_y, g_z$ are the gravitational acceleration vector components in the respective coordinate directions.

However, in a cylindrical geometry additional terms in the momentum balance arise that are dimensionally equivalent to body forces, (see Appendix A); these “equivalent” body forces are given by:

$$\bar{B} = \begin{pmatrix} -\sigma_{\theta \theta} / r \\ \sigma_{r \theta} / r \\ 0 \end{pmatrix}$$ \hspace{1cm} \text{Equation 22}$$

where $\sigma_{\theta \theta}$ is the normal stress in the theta (circumferential) direction and $\sigma_{r \theta}$ is the shear stress in the r-theta plane and these forces contribute to the relationship between radial and angular deformations. In the experiment that succeeded in producing the desired conceptual behaviour, the tensor $\bar{B}$ was set to zero despite a cylindrical geometry being used. Whilst $\bar{B}$ equals zero, the definitions of $\sigma_{\theta \theta}$ and $\sigma_{r \theta}$ remain unchanged (Howell et al, 2009). This change has no impact on the mass or volume conservation of the system, and Newton’s Second Law is still obeyed. This change does alter the way forces are created in a cylinder but hoop stresses are still generated through other terms in the cylindrical formulation (see Appendix A). Coupled with the pre-existing tensile failure rule, this alternative model enables the outer parts of the modelled bentonite to expand more easily, reducing the coupling between the inner and outer parts of the cylindrical system.

This is an interesting observation, consistent with the results of the BExM approach, which emphasises that the bentonite behaviour is very non-elastic, and much of the behaviour is highly plastic or indeed partially fluidic.

Using this adaptation of the equations to model the in situ experiment gives a significantly better fit both to the pressure at the tunnel wall at the sides and the top of the heater, where swelling into the void is most significant (Figure 4-11) and to the dry density distribution at the mid-length of the heater (Figure 4-12). The modelled pressure is now closer to that seen at locations 2, 3 and 4, which are the sides and the top of the tunnel, compared to location 1, which is at the base of the tunnel. This result is consistent with the modelling assumptions of a gap around the bentonite, which would not be present at the base of the tunnel, and also that the temperatures are representative of the sides and top of the tunnel rather than the bottom. The initial spike in the modelled total pressure represents the rapid increase in stress in the directions along the length of and
tangential to the container, due to swelling, followed by plastic failure in these directions. In the radial direction, stress gradually increases once the bentonite has swelled to fill the void space.

Data on dry density and water content are available after 5 years at the centre of Heater 1 and after 18 years at the centre of Heater 2. These data show that there was little change in dry density between 5 and 18 years and this is reflected in the QPAC model (Figure 4-12). The inner parts of the bentonite get wetter over this period both in the data and in the model (Figure 4-13).

This solution is highly specialised to a cylindrical geometry, but it provides another distinct avenue of investigation from the BExM and a much simpler resulting model.

Figure 4-10: Two conceptual models for how bentonite expands due to swelling in the outer portion. The top model represents the standard equations in which tensile stresses cause all compartments to expand. The bottom model represents the conceptual model tested in this variant case.
Figure 4-11: Pressure in the rock wall of the in situ experiment (Lanyon and Gaus, 2013) at locations shown in Figure 3-18, compared with the modelled pressure from the outer portion of bentonite, using updated ILM curves and including a void space and with the equivalent body force terms removed from the linear elastic equations. Note that both the total stress and the radial stress from the QPAC model are plotted.
Figure 4-12: Dry density in the in situ experiment (Lanyon and Gaus, 2013) at the central section of Heater 1 after 5 years and the central section of Heater 2 after 18 years, compared with the modelled dry density from the QPAC model with updated ILM curves, and including a void space and with the equivalent body force terms removed from the linear elastic equations.

Figure 4-13: Water content in the in situ experiment (Lanyon and Gaus, 2013) at the central section of Heater 1 after 5 years and the central section of Heater 2 after 18 years, compared with the modelled water content from the QPAC model with updated ILM curves, and including a void space and with the equivalent body force terms removed from the linear elastic equations.
4.5 Swelling model

The current swelling model is novel in that it considers swelling in the three coordinate directions (r, theta and z) separately and partitions the strain and water in each direction according to the current stress state in the three directions (see Section 2.5). This is in contrast to standard approaches in which the water content does not have a directional component. This approach, where the close association of the water and bentonite grains together with the stress field is more explicitly characterised, may represent the disposition of water within the bentonite grain structure more accurately. However, this type of approach is not yet widely adopted in the thermal-hydraulic-mechanical modelling community, where a simpler single-porosity based model of water content is preferred.. A consequence of this model is that the water content does not have any dependence on the history of the sample and is purely a function of current stress. The model behaviour is such that if, for example, the sample has swelled radially but then generated radial stress, the radial water content will increase with radial swelling and then decrease with radial stress. An alternative conceptual model is that the water content reflects both the current stress state and previous stress states such that increases in water content associated with swelling cannot be lost through increases in stress at a later time.

An alternative swelling model was implemented in QPAC, using the model in Section 4.4, in which the swelling strain is calculated as in Equation 17, but the water content in the three directions ($\omega_{nn}$ – see Section 2.4) is modelled as an evolving variable, with the change in amount of water ($Q$) in a given compartment taken from the hydraulic equations and then partitioned between the three directions based on the stress ($p'$ - total stress, $\sigma_{nn}$ - stress in normal direction n) at the current time in those directions:

$$\omega_{nn} = \int Q \left( \frac{p' - \sigma_{nn}}{2p'} \right) dt$$

Equation 23

This methodology bases the change in water content at a given time step on the stress whereas the previous method bases the instantaneous water content on the stress.

The updated model has the desired characteristic that water content in the r-direction remains higher than in the theta- and z-directions due to the swelling in the r-direction. However, this new model doesn’t show any significant improvement in terms of the pressure (Figure 4-14), dry density (Figure 4-15) and water content (Figure 4-16) over the previous model.
Figure 4-14: Pressure in the rock wall of the in situ experiment (Lanyon and Gaus, 2013) at locations shown in Figure 3-18, compared with the modelled pressure from the outer portion of bentonite, taken from the QPAC model with alternative swelling model.

Figure 4-15: Dry density in the in situ experiment (Lanyon and Gaus, 2013) at the central section of Heater 1 after 5 years and the central section of Heater 2 after 18 years, compared with the modelled dry density from the QPAC model with alternative swelling model.
Figure 4-16: Water content in the in situ experiment (Lanyon and Gaus, 2013) at the central section of Heater 1 after 5 years and the central section of Heater 2 after 18 years, compared with the modelled water content from the QPAC model with alternative swelling model.

4.6 Phase 2 Conclusions

The Phase 1 modelling showed that in broad terms, the ILM was able to reproduce the behaviour of laboratory experiments associated with the FEBEX programme and also results from the in situ FEBEX experiment. In Phase 2, improvements to this model were sought.

Significant improvement of the results was achieved by including the void space between the bentonite and the tunnel wall in the model and at the same time adapting the equations that describe elastic deformation of a solid. Addition of the void space alone resulted in minimal improvement, and without the void space, adapting the equations would have no effect. Conceptually, the effect of adapting the equations by removing the equivalent body forces is that bentonite is even further removed from being a standard elastic solid. Experiments have shown that bentonite behaviour is highly plastic or even partially fluidic (e.g. Millard et al., 2016), so adapting the equations and breaking assumptions about elastic behaviour seems reasonable.

Updating the ILM calibration had a small but positive effect on the fit of the model to the data. Using separate calibrations for the water retention curve and the swelling /
stress response of the bentonite means that the explicit link between hydraulic and mechanical properties used in the original ILM for MX80 bentonite/sand is weakened for FEBEX bentonite. However, the data that are required to calibrate these curves are generally available, so this is unlikely to affect the quality of predictions made with this model.

The updated swelling model did not significantly improve the results although it perhaps produced a conceptually more realistic solution.

Phase 1 modelling showed that with very few modifications, the ILM s set up for the SEALEX experiments could be directly applied to the FEBEX data and produce good fits to the data. In Phase 2, more significant updates to the ILM were considered to make improvements in the calibration of the model. These updates were focussed towards improving the mechanical model in order to produce better matches of the dry density distribution through the bentonite. An improved model was developed by explicitly including the void space between the bentonite and the tunnel and also adjusting the elastic equations to remove some of the equivalent body forces. Whilst this model is significantly better at reproducing the experimental observations than the previous models documented in this report, there are some uncertainties in interpretation of removing the equivalent body forces. However, the fact that such a change improves the modelling results does illustrate how different bentonite is from a classical poro-elastic medium and would provide an interesting avenue for future investigation to produce simpler, but effective models of bentonite – noting that the results achieved using this approach are comparable to those produced by the BExM, in terms of the fit of the model to the experimental data.
5 Conclusions

Quintessa has previously developed a model called the Internal Limit Model (ILM) to represent an MX80 bentonite and sand mixture that was used in the SEALEX experiments at the Tournemire URL. In modelling for RWM as part of the DECOVALEX-2015 project, the ILM was successful in reproducing observations from the SEALEX experiments. The FEBEX-DP project provided an opportunity to test the ILM on a different set of experiments and with a different bentonite. FEBEX-DP also provided a dataset against which updates to the ILM approach could be tested.

The ILC was calibrated to FEBEX data, and whilst the relationship between suction and swelling/consolidation seemed less strong than in the SEALEX experiment, a curve was calibrated to the three data sets and then used in modelling. A single parameter set for the ILM was sought by calibration against four laboratory experiments and the in situ experiment. To a large extent, this was achieved, although there are some notable exceptions, including the parameterisation of permeability for different experiments. This indicates that there is still some work required to produce models that are capable of reliable prediction without the need for significant calibration, but the work documented here is a step forward over modelling attempts with new parameter sets required for each experiment modelled.

Some consistent disagreements between the model and the experimental data have been noted across different experiments in Phase 1, and were the focus of further work in Phase 2. A number of cases showed the model over-predicting swelling pressures (e.g. constant temperature infiltration with loss of confinement and the 1D in situ model) and under-predicting volume of swelling (laboratory oedometer tests and the dry density distribution for the 1D in situ model). Two possible reasons for these observations are; that the ILM curves require an alternative calibration; and the swelling model needs further refinement.

For the model of the in situ FEBEX experiment, improvement to the model was made by the inclusion of the void space and adjustment of the equations that describe elastic deformation, suggesting that the bentonite behaviour is highly plastic or even partially fluidic. This update would not affect the models of the laboratory experiments since none of the experiments considered radial expansion into a void space. This does demonstrate the need for laboratory experiments that consider the same range of processes and geometries as are expected to occur at the field scale if laboratory data are to be used to as a basis of predictions. In particular, since many disposal concepts involve radial swelling of bentonite to fill near-circular tunnels, laboratory experiments must consider cylindrical geometries so that the appropriate mechanical processes are measured. Bentonite behaves differently to an elastic medium but this can only be
readily observed in experiments when bentonite swells into a void with a radial geometry.

This project has shown that with minimal calibration, the ILM that was set up for an MX80 bentonite and sand mixture can be applied to FEBEX bentonite in a suite of laboratory and field scale experiments and produce results that broadly reproduce the data. With some additional work, the ILM was able to produce a better fit to the experimental data. The major update to the ILM involves removing equivalent body forces when the geometry of the system involves radial expansion. This is an interesting concept because it implies that bentonite shows very little classical elastic behaviour which could lead to alternative conceptual models for representing bentonite. The ILM and investigations into the non-elastic behaviour of bentonite provide an alternative modelling concept to the widely used BBM and BExM models, which focusses on improving conceptual understanding of the bentonite rather than simply calibrating models to fit data.
6 References


Lanyon GW and Gaus I (2013). Main outcomes and review of the FEBEX In Situ test (GTS) and Mock-up after 15 years of operation. Nagra report NAB 13-96.


Appendix A

The strains and stresses in an elastic material are connected by a linear relationship (a generalisation of Hooke’s law), which is implemented in the QPAC mechanical module as follows (Howell et al., 2009):

\[ \sigma_{ij} = S_{ijkl} \varepsilon_{kl} \]

where \( S_{ijkl} \) is the elastic stiffness tensor (Pa), \( \sigma_{ij} \) is the Cauchy stress tensor (Pa) and \( \varepsilon_{kl} \) is the strain tensor (\( \cdot \)). The tensor indices \( i,j,k,l \) all have a range from 1 to 3 in three dimensions, and the summation convention has been used to omit explicit sums over \( k \) and \( l \). In this formulation, strain is defined as follows:

\[ \varepsilon = \frac{1}{2} ( \nabla \vec{u} + \nabla \vec{u}^T ) \]

where \( \vec{u} \) is the three-dimensional displacement vector (m).

In practice, due to considerations of symmetry, this relationship can be simplified by changing the upper diagonal of the strain and stress tensors into a six-row vector, with consequent simplification of the stiffness matrix to a second order, rank 6 tensor. For applications to soil mechanics it is also typical to include strains for plasticity and thermal expansion effects (\( \gamma \)), and the pore pressure \( P \) (MPa), following effective stress theory (Jaeger et al., 2007):

\[ \bar{\sigma} = S ( \bar{\varepsilon} - \bar{\gamma} ) - P \]

The overall conservation relationship is via momentum conservation as:

\[ \rho \frac{\partial^2 \vec{u}}{\partial t^2} = \nabla \bar{\sigma} - \vec{B} \]

where \( \vec{B} \) is the body force per unit volume (N/m\(^3\)) and \( \rho \) is the density (kg/m\(^3\)). Body forces act across the whole volume of the solid rather than being applied at surfaces (tractions); examples of a body force would be the forces arising due to the local acceleration due to gravity, or a centripetal acceleration.

From Howell et al., (2009 – equation 1.11.3) the expanded form of the momentum conservation equation in a Cartesian system is:

\[ \rho \frac{\partial^2 u}{\partial t^2} = \rho g_x + \frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} + \frac{\partial \sigma_{xz}}{\partial z} \]

\[ \rho \frac{\partial^2 v}{\partial t^2} = \rho g_y + \frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} + \frac{\partial \sigma_{yz}}{\partial z} \]

\[ \rho \frac{\partial^2 w}{\partial t^2} = \rho g_z + \frac{\partial \sigma_{xz}}{\partial x} + \frac{\partial \sigma_{yz}}{\partial y} + \frac{\partial \sigma_{zz}}{\partial z} \]

where \( (u,v,w) \) are displacements in the Cartesian directions, and the gravitational acceleration terms \( (\rho g_x, \rho g_y, \rho g_z) \), if non-zero, make up the \( \vec{B} \) vector.
The equivalent equations in cylindrical coordinates \((r, \theta, z)\) are (Howell et al., 2009; equation 1.11.7):

\[
\rho \frac{\partial^2 u_r}{\partial t^2} = \rho g_r + \frac{1}{r} \frac{\partial}{\partial r}(r \sigma_{rr}) + \frac{1}{r} \frac{\partial \sigma_{r\theta}}{\partial \theta} + \frac{\partial \sigma_{rz}}{\partial z} - \frac{\sigma_{\theta\theta}}{r}
\]

\[
\rho \frac{\partial^2 u_\theta}{\partial t^2} = \rho g_\theta + \frac{1}{r} \frac{\partial}{\partial r}(r \sigma_{r\theta}) + \frac{1}{r} \frac{\partial \sigma_{\theta\theta}}{\partial \theta} + \frac{\partial \sigma_{\theta z}}{\partial z} + \frac{\sigma_{r\theta}}{r}
\]

\[
\rho \frac{\partial^2 u_z}{\partial t^2} = \rho g_z + \frac{1}{r} \frac{\partial}{\partial r}(r \sigma_{rz}) + \frac{1}{r} \frac{\partial \sigma_{\theta z}}{\partial \theta} + \frac{\partial \sigma_{zz}}{\partial z}
\]

Comparing the cylindrical and Cartesian versions of the momentum equation, for a cylindrical geometry there are additional components in the momentum balance equation that are dimensionally equivalent to body forces and outside of the stress spatial derivative terms. In the QPAC formulation these additional terms that arise due to the geometry and the elasticity, are included directly in the body forces vector:

\[
\vec{B} = \left( \begin{array}{c} -\sigma_{\theta\theta}/r \\ \sigma_{r\theta}/r \\ 0 \end{array} \right)
\]

The fact that these terms appear separately from the definitions of stress and strain and only in the momentum balance, means that they have no direct impact on continuity; they only adjust the force balance across a body.