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ORIGINAL PAPER

Coupled Hydromechanical Modelling of a Vertical Hydraulic Sealing System Based on the Sandwich Principle

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Abstract

For the shaft sealing of a repository for radioactive waste, a Sandwich sealing system was developed by KIT-CMM consisting of bentonite-based sealing segments (DS) and sand mixture-based equipotential segments (ES). To demonstrate the functionality of the Sandwich sealing system, various laboratory tests (MiniSandwich tests and semi-technical scale experiments) have been carried out before a large-scale experiment has been implemented in situ at the Mont Terri Rock Laboratory (CH). An important coupled process in the Sandwich system is the swelling deformation of the DS while aqueous fluid penetrates into the system. Consequently, the interparticle porosity (effective porosity) of the DS decreases by swelling strain, resulting in a reduction in the permeability of the DS. Pore space of the ES also decreases slightly due to swelling stress in the adjacent DS, which also leads to a reduction in the permeability of the ES. To understand the coupled hydromechanical processes of the Sandwich sealing system, a numerical model was developed to interpret the experimental observations from the MiniSandwich tests and to parameterize different components. A linear swelling model for DS and empirical functions for the swelling deformation-induced permeability change for both DS and ES segments were introduced into the coupled model with Richards' flow and elastic model. Sensitivity analysis with parameter variations of the most important parameters reduces the uncertainty in the system behavior.

Highlights

- The Sandwich concept is an innovative idea for realizing the sealing effect in a repository for radioactive waste.
- The MiniSandwich experiments are carried out under well-defined conditions and reveal the hydromechanical responses in the Sandwich system and provide a high-quality database.
- A simple emperical model based on physical observations was developed to simulate the measured flow and stress and to account for the interaction between sealing segment (DS) and equipotential segment (ES).
- In this model, swelling-induced permeability change for DS and compaction-induced permeability change for ES are intensively studied.

Keywords Shaft sealing · Sandwich system · MiniSandwich experiment · Coupled hydromechanical modelling · Numerical code OpenGeoSys (OGS)

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1 Introduction

Geotechnical barriers in a repository for radioactive waste include the sealing of boreholes, drifts, and shafts closures. As the final construction project, the shaft sealing plays an important role in the entire multi-barrier system. In various international concepts, bentonites are considered as a favorable sealing material in all types of host rocks, especially in crystalline and clay rock. Bentonite-based seal concepts commonly consist of a static abutment and a sealing core (Emmerich et al. 2019). Due to its swelling capacity, bentonite, especially Na-rich bentonite, expands in contact with water and generates a swelling pressure that leads to an increase in the interlayer porosity and a reduction in the interparticle pore space and permeability, but, excessive swelling pressure can cause the surrounding rock to fail. Various variants were tested internationally in underground facilities. Quite often a bentonite/sand mixture is used as backfill material. Bentonite/sand mixtures with different mixture ratios (40/60, 30/70) have been extensively tested in the Whiteshell Laboratory, Canada (Dixon et al. 2017). Clay pellets/powder from the Paris Basin were used for shaft and borehole sealing at HADES URL, Belgium (Van Geet et al. 2009). A summary of several experiments performed so far with detailed information can be found in Emmerich et al. (2019).

Uniform wetting of the bentonite is the prerequisite for high functionality and performance. Still, fingering is a known phenomenon in soil physics that leads to an accelerated water flow along preferential pathways later followed by a water break through and inhomogeneous swelling of the bentonite. To reduce preferential flow inside the conventional mixture seal system as well as bypass along the contact zone to the host rock and the excavation damaged zone (EDZ) especially in clay rock, a promising concept for seal elements, the Sandwich system, was developed by Karlsruher Institut für Technologie (KIT) (Nüesch et al. 2002, Emmerich et al., 2019). The respective seal consists of alternating segments of bentonite-based sealing segments (DS) and sand mixture-based equipotential segments (ES) with higher hydraulic conductivity to promote a homogeneous hydration and swelling process (Fig. 1).

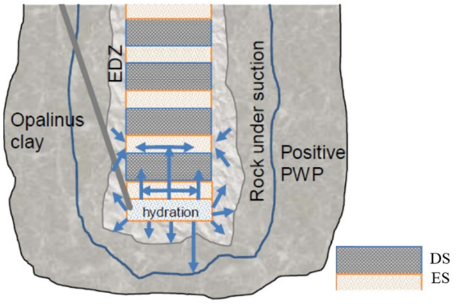

Fig. 1 A conceptual layout of a Sandwich sealing system in a shaft in clay rock

To demonstrate the functionality of this system and to understand the coupled hydromechanical processes, various laboratory tests (MiniSandwich tests and semi-technical scale experiments) were carried out. A large-scale experiment in situ is being carried out at the Mont Terri Rock Laboratory (CH) (Emmerich et al. 2019). The long-term measurement data from the laboratory tests provide valuable information on the hydromechanical and geochemical behavior of the sealing system. Numerical evaluation of the semi-technical scale experiment and even the large-scale in situ tests requires a sufficient understanding of the underlying material processes, e.g., swelling and the corresponding permeability decrease associated with geochemical changes, as well as a calibrated material parameter base. Therefore, the MiniSandwich tests (Emmerich et al. 2021) under well-controlled test conditions provide all the important information for model validation and parameter calibration of such a complicated system.

A coupled hydromechanical code is essential for modelling the bentonite sealing system. In this general hydromechanical algorithm, particular care must be taken with the change in hydraulic parameter caused by swelling. The swelling pressure increases with an increase in the dry density and decreases with an increase in the salinity of the solution (Pusch 1980; Gens and Alonso 1992; Xie et al. 2007). The current swelling pressure models can be divided into three groups: double-layer models, thermodynamic models and empirical models based on the experimental results. Most models assume no volume change. Some publications show the swelling model under volume change (e.g., Cui et al. 2002). We will not follow the hydrochemical aspects and focus on the hydromechanical mechanism in this study. A widely used model for bentonite material is the Barcelona Expansive Model (BExM) (Alonso 1999) to describe the coupled hydromechanical behaviour of the double porosity mixture (micro and macro-porosity). BExM considers the distinction of the deformational response of these two porosity levels, which are affected by mean net stress and suction changes (macro-porosity) and mean effective stress changes (micro-porosity). However, a number of parameters associated with BExM are needed for describing both elastic and plastic behavior (Alcantara et al. 2020), which must be calibrated by using different experimental data. Sufficient data, in particular for the two bentonites Calcigel and Secursol UHP used in this study, are not yet available. Moreover, more effort is required to apply this model in this composite system made of two different materials DS and ES.

Since the volume changes in both DS and ES are undefined and do vary during the hydration process, the available

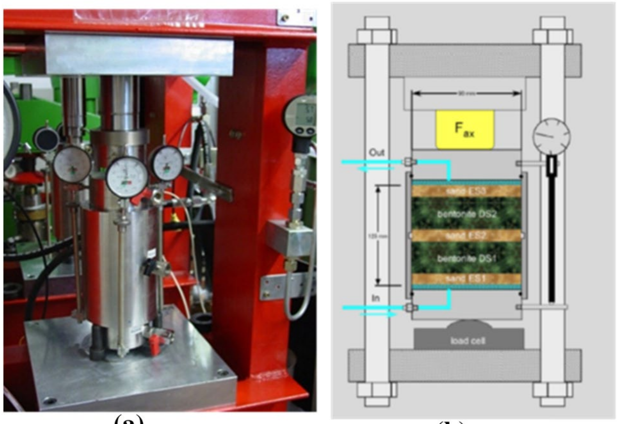
(a) (b)

Fig. 2 **a** Customized oedometer apparatus used for the MiniSandwich experiment and (b) Sketch of the experimental layout (Roelke et al. 2019; Emmerich et al. 2019)

models can only be used to a limited extent. In this paper, we present a simplified model based on the coupled multiphysics code OGS (Kolditz et al. 2012) to simulate the experimental observations in the MiniSandwich, with a focus on the interaction between DS and ES generated by water infiltration into the clay-rich material DS. The suggested simplification is that the hydration-induced change in hydraulic parameters is described by an empirical permeability-deformation function for both DS and ES. The focus of the model is therefore on the hydraulic process apart from the mechanical effect on the porosity change.

The general objectives of the simulation of the MiniSandwich experiments can be summarized as follows: (1) Identification of coupled hydro-mechanical processes in the Sandwich sealing system, considering the interaction between DS and ES. (2) parametrization of individual components and determination of the material parameter of the Sandwich sealing system, and (3) interpretation of the long-term experiment and evaluation of the behavior of the overall system (Sandwich sealing system and Opalinus Clay) behavior.

2 Laboratory MiniSandwich Experiment

The MiniSandwich tests, a series of tests in a customer-specific oedometer device (Fig. 2a), were carried out in the IfG rock mechanical laboratory (Roelke et al. 2019). The MiniSandwich specimens consist of two DS sandwiched by three ES (fine sand) (Fig. 2b). Two German Ca-rich bentonites (Calcigel and Secursol UHP/sand mixture) as DS, different injection fluids (4 M NaCl brine and Pearson water from the Mont Terri Rock Laboratory, NAGRA 2002) at different injection pressures and different initial saturation states were tested to analyze the mechanical and chemical reactions. Extensive data sets are available from the well-controlled experiments.

The small-scale tests with a diameter of 90 mm and a volume of approximately 800 cm^3 measure the swelling and fluid flow parameters on well-prepared sample assemblies (Fig. 2). The modified oedometer cells were constructed as steel tubes with two movable pistons and filter plates for adjusting well-defined saturation conditions (Popp et al. 2015). The cells were located in hydraulic load frames. The axial strain during swelling of the specific bentonite material was measured by three gauges (displaced by 120°). During the test, the axial strain was regularly reset to zero by increasing the axial load measured by a load cell under quasi-constant volume conditions. During saturation, the fluid volume balance was monitored and the stationary fluid permeability was calculated. The liquid was collected at the outflow (top) and analyzed to study ion transport and cation exchange processes (Emmerich et al. 2019).

In the first test series, tests on two bentonite materials (Calcigel and Secursol UHP) were performed under different test conditions (0.1 and 0.3 MPa injection pressure) and different fluids (NaCl water and Pearson water) for hydration. The two tests (Oe8 and Oe10) were selected and interpreted by numerical simulation in this study because both of them were tested using Pearson water from Mont Terri Rock Laboratory (pore fluid of Opalinus clay (Pearson et al. 2003). In the test Oe8, Calcigel bentonite with a smectite content of 64% (Emmerich et al. 2021) with a dry density of 1.55 g/cm^3 and an initial water content of 11.2% by weight was used as DS. The ES segment (fine sand N45) was installed with a density 1.56 g/cm^3 (Emmerich et al. 2009). Pearson water with an injection pressure of 0.1 MPa was used as the hydration fluid. The total porosity accessible to gas was 37.7% and the total system gas permeability was 4.5E−14 m. The porosity was calculated using dry density and specific density. The gas permeability was determined in a steady-state flow test with technical nitrogen in oedometer cells. All values were determined in the IfG laboratory (Emmerich et al. 2021). The swelling pressure of the entire system was measured at 1.2 MPa. These parameters were the initial values for the numerical modelling. The test was terminated after about 430 days because there was still no fluid outflow. All segments were sampled and analyzed after dismantling. The result showed that the ES1 (lowest ES layer) was completely saturated ($w = 26.2\%$) and the DS1 and DS2 layers had a water content ranging from 27 to 33%. The ES2 and ES3 layer were mostly dry ($w = 0.08$–0.73%) (Roelke et al. 2019; Emmerich et al. 2019).

The raw material Secursol UHP has a relatively high smectite content of 79%, which is characterized by a very high swelling pressure of > 4 MPa at a dry density of about 1.55 g/cm^3. Therefore, the bentonite was mixed with fine sand N45 to reduce its smectite content, and thus its swelling

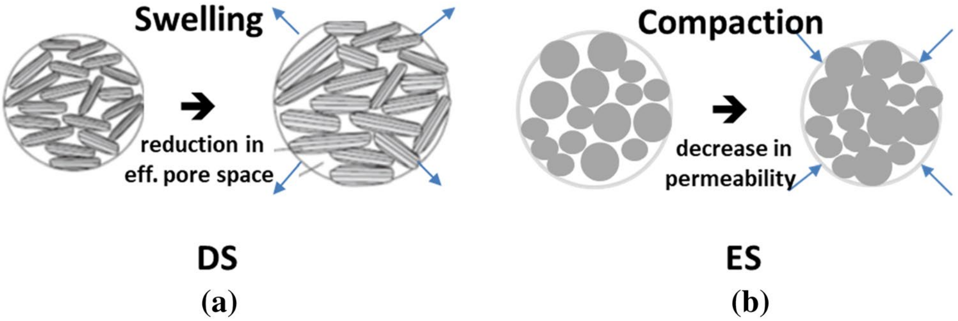

Fig. 3 Microstructure change of DS due to swelling (**a**) (modified from Xie et al. 2006) and of ES due to compaction (**b**)

pressure (Emmerich et al. 2021). In the test Oe10, mixtures of Secursol UHP and fine sand with a mixing ratio of 1:0.28 were used for the DS to achieve an EMDD (effective montmorillonite dry densit) similar to the Calcigel used in Oe8. The resulting dry density of the DS was 1.33 g/cm^3. The gas-accessible porosity was relatively high (46.5%) and the gas permeability was 5.6E−12 m^2. The initial water content of 12.9% by weight was measured. Pearson water was injected at 0.3 MPa, which is higher than the injection pressure used in the Oe8, and fluid breakthrough occurred in less than 20 days, resulting in nearly steady-state flow conditions. The same effective montmorillonite dry density of both tests should present similar hydro-mechanical behavior, but the high injection pressure and the addition of fine sand in the DS in Oe10 accelerated liquid breakthrough (Emmerich et al. 2019).

3 Analysis of Coupled Processes in the Sandwich Sealing System

An important coupled process in the Sandwich system is the swelling deformation of the DS while aqueous fluid penetrates into the system.

Both DS and ES are implemented quite homogeneously in the MiniSandwich device. The ES has a fairly high initial permeability, so water can easily flow into the ES1 and shortly thereafter the ES1 is fully saturated with water up to the top of the ES1 where DS1 is placed. The bentonite (DS) has a high suction and sucks the water up into the interface between DS1 and ES1.

Due to the relative low permeability of the DS, and in particular the swelling capacity, water is adsorbed in the interlayer of the smectite and the smectite swells. The swelling deformation leads to a reduction of the interpartical pore space (effective porosity) in the DS (Fig. 3a), because the volume of the overall system is laterally limited. The reduction of the pore space leads to a decrease in the permeability of the DS, consequently water infiltration throughout the DS is slowed down.

Swelling deformation is still possible in the longitudinal direction, which results in a compaction stress on the adjacent ES in both directions, upwards, where ES2 is located, and downwards (ES1). Under the compaction stress, the pore space of the ES also decreases slightly, which additionally leads to a small reduction in the permeability of the ES (Fig. 3b).

To simulate this interaction between DS and ES, a linear swelling model describing the linear relationship between swelling stress and water saturation for bentonite and an empirical permeability-strain function are introduced into Richards' flow-elastic coupled hydromechanical model.

4 Numerical Model and Realization

To simulate complicated phenomena, a numerical model capable of handling the coupling process is indispensable. The basis of the theoretical framework is the coupled hydro-mechanical process, which is based on balance equations and constitutive relations. Due to the low gas pressure in the system, we use Richards' approximation to treat the flow problem in partially saturated and even unsaturated deformable porous media.

4.1 Mass balance in terms of Richards' flow

The mass balance equation in terms of Richards' flow in the deformable porous media DS and ES can be expressed as:

$$\frac{\partial}{\partial t}(nS^w\rho^w) + \nabla\mathbf{q}^w + nS^w\rho^w\nabla\frac{\partial\mathbf{u}}{\partial t} = Q^w \tag{1}$$

where n is the porosity of the medium, ρ^w denotes the density of water, $\mathbf{u}$ is the displacement vector, Q^w is the source or sink term. q^w is the advection of water flow, which is described by Darcy's equation:

$$\mathbf{q}^w = -\rho^w\frac{\mathbf{k}k^w_{rel}}{\mu^w}(\nabla p^w - \rho^w\mathbf{g}) \tag{2}$$

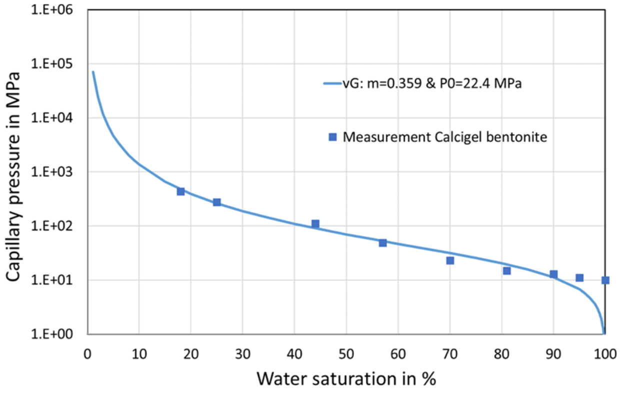

Fig. 4 Fitting of the Van Genuchten function to Calcigel bentonite (Data from Emmerich et al. 2019)

where **k** is the intrinsic permeability matrix, k^{w}_{rel} is the relative permeability to water, μ^{w} is the water viscosity, and **g** is the gravity vector.

In the case of Richards' flow model, the gas pressure is zero, so the capillary pressure can be expressed as negative water pressure, indicating the unsaturated state. We use the van Genuchten function to describe the suction behavior of bentonite:

$$p^{c} = p^{0}\left[S_{eff}^{-1/m} - 1\right]^{(1-m)} \tag{3}$$

where p^0 is the air entry pressure, m is the dimensionless pore size distribution index. S_{eff} is the effective saturation, which can be calculated as:

$$S_{eff} = \frac{S - S_{r}}{S_{\max} - S_{r}} \tag{4}$$

with S_{max} and S_r as the maximum and residual saturation, respectively. The van Genuchten function for the argillaceous material is highly nonlinear and requires an enormous amount of computation. The parameters in the van Genuchten function were fitted to the laboratory data of Calcigel bentonite (Fig. 4), and used to describe the retention behavior of the DS with a high suction capacity due to its smectite content.

4.2 Balance of Linear Momentum

Deformation processes in both DS and ES are described by the momentum balance equation based on Terzaghi's concept of effective stress extended by Bishop's model:

$$\boldsymbol{\sigma}_{ij} = \boldsymbol{\sigma}_{tot} - \alpha p^{w}(S^{w})^{\chi}\mathrm{I} \tag{5}$$

where $\boldsymbol{\sigma}_{tot}$ is the total stress vector. α is the Biot's coefficient used as a constant, p^w is the pore pressure, S^w is the water saturation, χ is the saturation-dependent effective stress parameter of Bishop's type (Nowak et al. 2011), **I** is the identity vector. Because the saturation changes during the hydration process, the effective stress will therefore change.

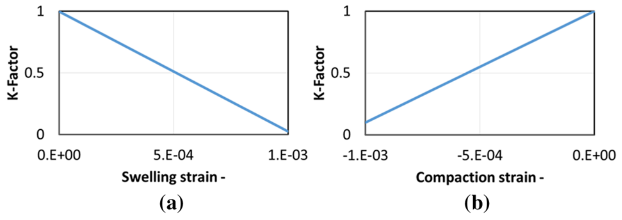

Fig. 5 Permeability model for the DS induced by swelling deformation (**a**) and ES induced by compaction deformation (**b**)

To describe the swelling or shrinkage behavior of DS depending on their moisture content, we introduce a linear swelling stress model similar to that used in Rutqvist et al. 2001:

$$\Delta\boldsymbol{\sigma}_{\mathrm{sw}} = -\boldsymbol{\sigma}_{\mathrm{max,sw}}\Delta S^{w}\mathbf{I} \tag{6}$$

$\boldsymbol{\sigma}_{max,sw}$ represents maximum swelling pressure and ΔS^{w} is the change in water saturation. The stress increment induced by swelling deformation is incorporated in the equation of balance of momentum as follows:

$$\nabla \cdot \left(\boldsymbol{\sigma}_{tot} - \alpha p^{w}(S^{w})^{\chi}\mathbf{I} - \boldsymbol{\sigma}_{sw}\right) + \rho \cdot \mathbf{g} = 0 \tag{7}$$

By applying the weighted residual method to the momentum Eq. (7), the total strain, which is equal to the elastic strain plus the swelling strain, is solved. The pore pressure p^w in Eq. (7) is the hydraulic primary variable and is solved in the mass balance equation coupled with Eq. (7). The water saturation S^w is determined by the suction curve at negative pore pressure (Eq. 3, Fig. 4).

For most materials used in geotechnical engineering, such as the ES segment, the solid grains are assumed to be incompressible, the mechanical deformation affects the change in porosity (pore space). In the case of swellable bentonite, such as the DS segment, the swelling deformation leads to a change in the porosity on the macro-scale (pore space) and also the porosity on the micro-scale (solid grains), so-called double-layer in the clayey material. The change in porosity leads finally to the change in permeability, which is more relevant to a hydraulic process. A very popular model for describing these changes is the double structure model BExM (Alonso et al. 1999). In this model, two porosities in the macrostructure and microstructure and their ratio should be considered and calibrated. In addition, the relationship between the porosity and permeability should be defined for each material used.

We try to skip these procedures to treat the porosity change and just consider the ultimate result about the permeability change of the system. As described in the

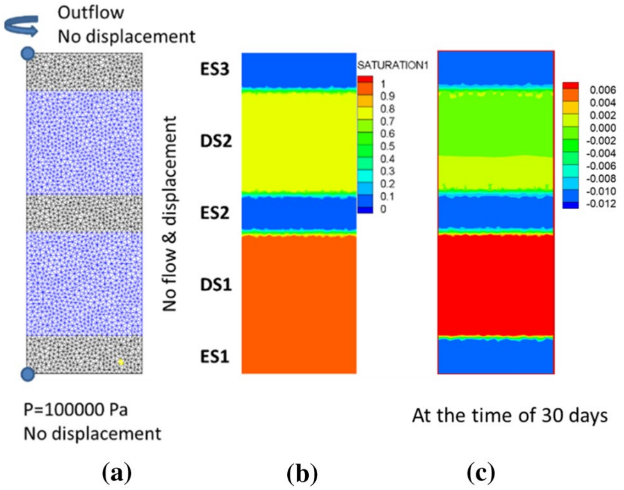

Fig. 6 Numerical model and boundary conditions (**a**), an example of the distribution of saturation indicating the suction effect of the DS (**b**), and strain distribution indicating the swelling expansion in DS and the compaction in ES (**c**) for Oe8

section above, an important process herein is the reduction in permeability due to the increase of swelling stress in the confined DS system. This reduction is represented by a linear relationship between permeability and swelling strain (Fig. 5a). At the same time, a linear relationship between permeability and compression strain is introduced to describe the change in permeability in the ES (Fig. 5b). Both relationships are empirical in a simplified form and only two parameters each need to be calibrated based on experimental data. In the linear relationship, the K-factor thresholds were tested extensively to fit the experimental data. Finally, a threshold value of 0.025 for the permeability function of swelling strain at a strain of per mill and 0.01 for the compaction strain is defined. Additionally, to prove the validation of the correlations for the Calcigel bentonite used, an extensive study including the data from swelling tests was carried out (Shao 2022b).

5 Model Calibration and Results

To optimize the test design in situ and to estimate the test duration, a numerical model with suitable parameters is essential. Many parameters for individual components are already known from literature studies and laboratory tests, e.g. the retention curve for Calcigel performed in the laboratory (Emmerich et al. 2019) (Fig. 4). In addition, however, we still have to describe the interaction processes in such a Sandwich sealing system. Therefore, a coupled hydro-mechanical model was developed to simulate the hydration process in the Sandwich system. In this model, both DS and ES were considered as a porous medium with different hydraulic and mechanical properties.

An axisymmetric 2D finite element mesh (Fig. 6a) for the OpenGeoSys (OGS) code (Kolditz et al. 2012), was constructed to simulate tests from the Pearson water series in the MiniSandwich experiment. Bentonite was installed with different initial water content (Oe8: 10.2% and Oe10: 12.9%) and dry density (Oe8: 1.55 g/cm^3 and Oe10: 1.33 g/cm^3) and therefore with different maximum swelling stresses (Eq. 6). A set of parameter values from the individual experiments

Table 1 Hydraulic parameter as reference for the MiniSandwich test Oe8 (Calcigel bentonite) and Oe10 (Secursol UHP with fine sand 1:0.28)

Parameter	Unit	DS (Oe8)	DS (Oe10)	ES (Oe8)	ES (Oe10)	Source
Permeability	m^2	2.50E−18	4.20E-17	1.30E-11	1.30E-11	Emmerich et al. (2019)
Porosity	[–]	0.5	0.5	0.4	0.4	Emmerich et al. (2019)
Rel. permeability		vG	vG	vG	vG	Fitting
Permeability–strain		Linear	Linear	Linear	Linear	Empirical
Entry pressure	MPa	9	9	0.1	0.1	Assumption
vG shap factor	[–]	0.5	0.5	0.5	0.5	Fitting
Residual saturation	[–]	0	0	0	0	Assumption
Maximum saturation	[–]	1	1	1	1	Assumption

Table 2 Mechanical parameter as reference for the MiniSandwich test Oe8 ($\rho_d = 1.55$ g/cm^3) and Oe10 ($\rho_d = 1.33$ g/cm^3)

Parameter	Unit	DS (Oe8)	DS (Oe10)	ES (Oe8)	ES (Oe10)	Source
Young‘s modulus	GPa	0.15	0.15	0.3	0.3	Ref. to other bentonite
Poisson‘s ratio	[–]	0.15	0.15	0.2	0.2	Assumption
Density	kg/m^3	1600	1600	1500	1500	Emmerich et al. (2019)
Biot number	[–]	0.6	0.6	0.6	0.6	Other study
Bishop coef.	[–]	1.4	1.4	1.4	1.4	Other study
Max. swelling stress	MPa	3.5	2.1	–	–	Emmerich et al. (2019)

and the literature was used as the basic parameter for the first calculation. The most important factors influencing this strong hydromechanical coupling are the permeability and Young's modulus and the permeability-strain-relationship. Therefore, these parameters are varied extensively until a reasonable result is obtained, e.g. permeability for DS (6.44E−18 ~ 2.5E−18 m^2) and ES (5E−14 ~ 1.3E−11 m^2), retention curve parameters, Young's modulus (0.1 ~ 0.5 GPa), swelling pressure (0.7 ~ 3.5 MPa), Poisson's ratio (0.1 ~ 0.4), porosity, and permeability-strain-function for both materials. This job also serves as a sensitivity study. Finally, in Table 1 (hydraulic parameter) & Table 2 (mechanical parameter) a reference parameter set for the MiniSandwich test with Calcigel bentonite and with Secursol/sand mixture is presented. The high permeability of DS in the Oe10 is due to the addition of sand to the Secursol bentonite (Table 1) and the low swelling pressure is due to the low dry density used in Oe10.

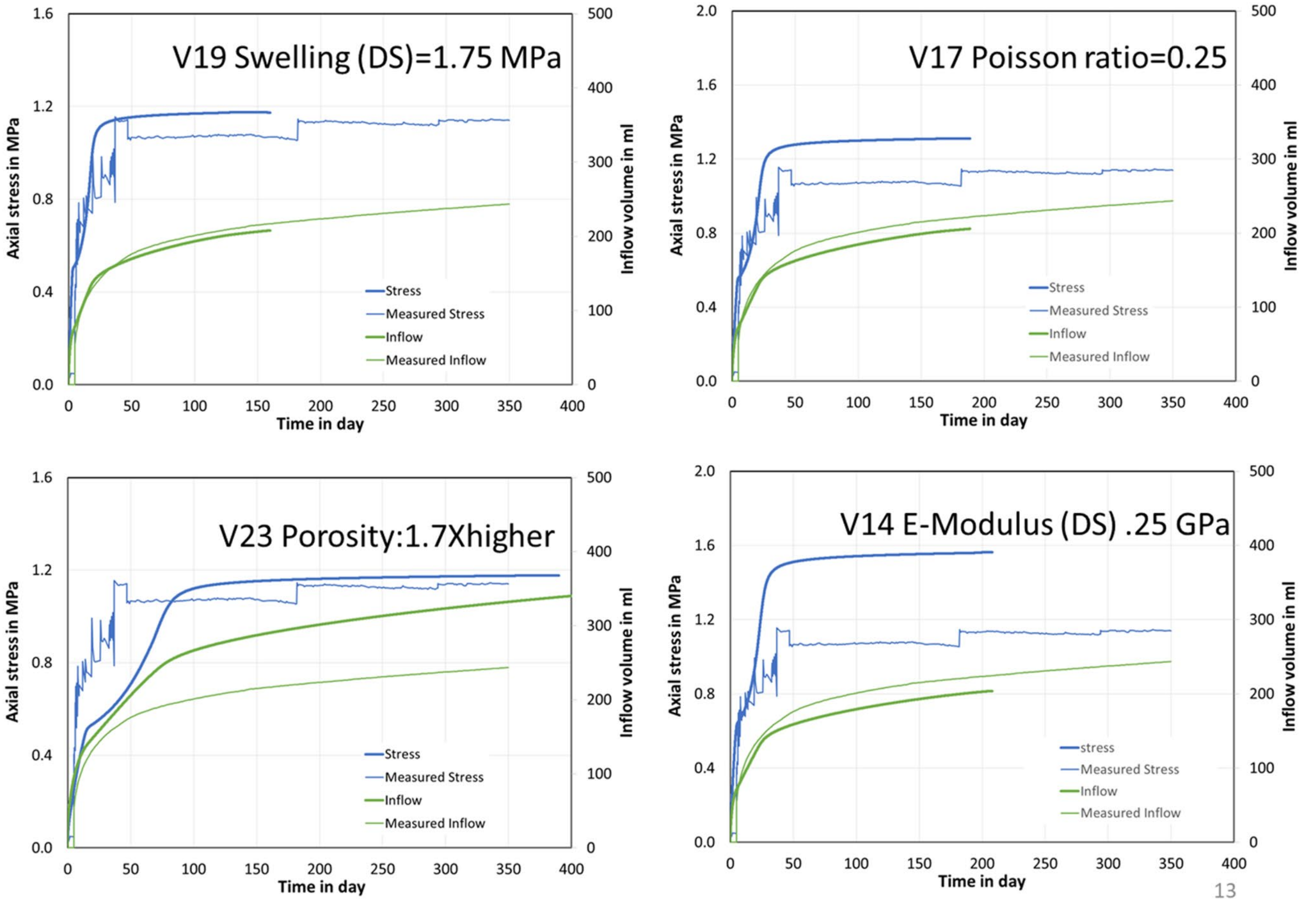

Fig. 7 Sensitivity analysis of some key parameters (Table 3) for test Oe08 (MiniSandwich test with Calcigel bentonite)

Table 3 Varied parameter used in the Fig. 8 (V20 is the reference case)

Variation	ES				DS				Swell. pressure
	Permeability	Porosity	Young's modulus	Poisson	Permeability	Porosity	Young's modulus	Poisson	
	m²	[–]	GPa	[–]	m²	[–]	GPa	[–]	MPa
V14	1.30E–11	0.4	0.30	0.35	2.50E–18	0.5	0.25	0.42	1.75
V17	1.30E–11	0.4	0.30	0.25	2.50E–18	0.5	0.15	0.25	1.75
V19	1.30E–11	0.4	0.30	0.23	6.40E–18	0.5	0.15	0.23	1.75
V20	1.30E–11	0.4	0.30	0.2	2.50E–18	0.5	0.15	0.15	3.5
V23	1.30E–11	0.68	0.30	0.2	2.50E–18	0.85	0.15	0.15	3.5

To simulate the Oedometer experiment, no lateral displacement and no flow condition at the radial boundary were set due to a rigid confining ring. In the vertical direction, however, the axial strain and the axial stress may change due to swelling. If there is no vertical strain, a zero displacement is set at the top of the model. But, this theoretical zero cannot always be realized in the experiment. As described in the section, the axial strain was regularly reset to zero by increasing the axial load measured by a load cell under quasi-constant volume conditions. In the Oe8, the total strain deviation was low in a range below 0.01%, therefore, a condition with no axial displacement can be used (Fig. 6a). However, large deformation was observed in the Oe10, especially on day 70, a sudden system change (strain deviation of 0.79%) will cause a stress drop, after adjustment, the axial stress will stepwise increase to the original value. As a boundary condition at the top of the sample, a time-dependent strain is used for the case Oe10 (Fig. 9). Due to this fact, the measured stress is only used for trend and magnitude, especially the reaction to the deformation. The injection area was defined at the bottom with an injection pressure of 0.1 MPa for Oe8 and 0.3 MPa for Oe10. The drain was at the top of the model.

The results (Fig. 7) show that the characteristic pattern of the total stress development, which is very similar to a typical swelling test on a homogeneous swelling material, does not change significantly. More variations with parameter combination can further improve a better fit to the experimental data and, therefore, optimize the parameters for each material. The specified set of parameters and this range can cover the uncertainty of the system. The simulated saturation distribution, where DS2 saturates first before ES2 and ES3 saturate, is qualitatively consistent with the observation (Fig. 6b). Figure 6c shows the total strain in the system on day 30. While the DS is loaded by swelling under expansion strain (represented in positive), the ES shows compaction strain (represented in negative). Both swelling expansion and compaction lead to a permeability reduction in the DS and ES, respectively. A thin layer from expansion to compaction can be observed in the transition zone between DS and ES.

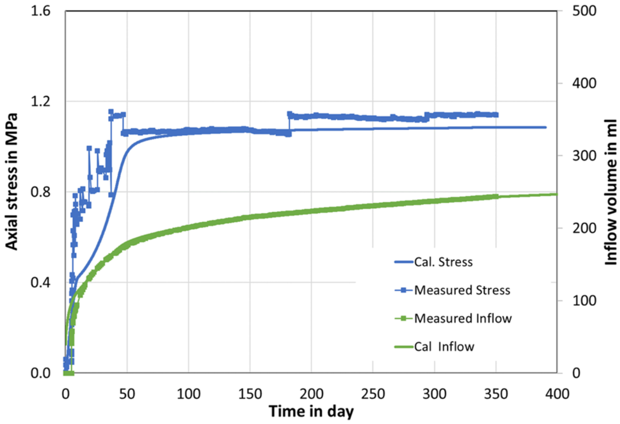

Fig. 8 Stress and flow evolutions of test Oe08 (MiniSandwich test with Calcigel bentonite)

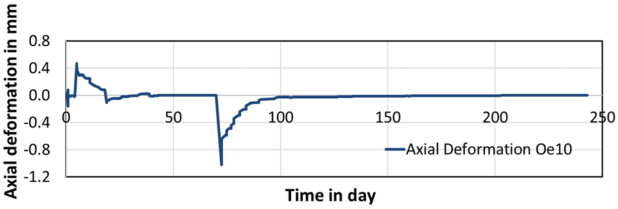

Fig. 9 Measured axial deformation of the Oe10 test as a numerical boundary condition

Figure 8 shows both the stress and the inflow evolutions for Oe8 with the best combination of parameters (reference values in Tables 1 and 2) so far. The calculated inflow agrees quite well with the measured data, showing that the permeabilities of DS and ES from the swelling and the compaction deformation are well estimated. Based on Fig. 5, both permeabilities are reduced to one percent of the original, so two orders of magnitude smaller. Most water (181 ml: 70% of the total measured inflow over the first 350 days) entered the system during the first 50 days, indicating that the ES1 and DS1 was fully saturated. The accessible volume of these three elements is calculated to be 191 ml without considering the change in porosity. Thereafter, the increase in inflow is very slow, indicating a preventive functionality of the DS2 (Fig. 10)

A slight underestimation of the total stress can still be observed. Both calculated trends (total stress and inflow) agree fairly well with the measurement. In particular, the concave increase in total stress during the first 50 days and the slight increase thereafter can be captured numerically. This concave increase is consistence with the increase in water in DS1. On day 37, the stress reached a maximum. The high swelling stress compacts the adjacent ES, and the pore structure of the ES may rearrange, resulting in lower stress. After that, the gradual increase in stress in the late phase indicates slow water uptake in DS2.

A similar model was used for the test Oe10, but with a different test height (0.13 m instead of 0.125 m for Oe8). The parameters used for Oe8 were also used for Oe10, but taking into account the higher injection pressure with 0.3 MPa and the lower dry density (low swelling capacity) for DS with 1.33 g/cm^3. The latter can lead to an increase in permeability and a reduction in the maximum swelling pressure. These two parameters were therefore varied intensively. Deviating from Tables 1 and 2, the permeability is finally set at 4.2e−17 m^2 and the maximum swelling pressure at 2.1 MPa for DS. As expected, a very fast breakthrough was simulated without observing a typical stress development like in case

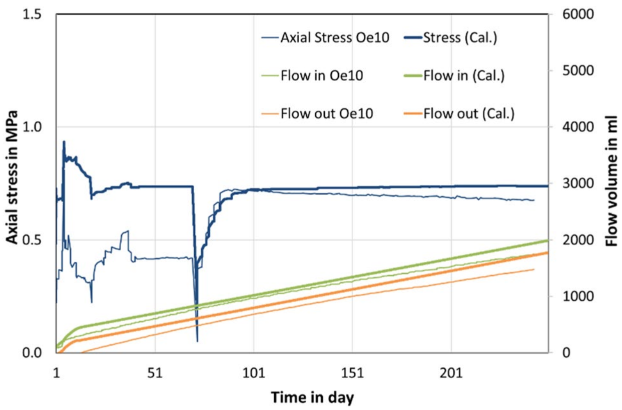

Fig. 10 Stress and flow evolutions of test Oe10 (MiniSandwich tests with Secursol)

Oe8 (Fig. 10). The calculated difference between the inflow and outflow is about 230 ml (276 ml in the measurement).

A fairly good parameter set was obtained in the MiniSandwich experiment for both DS and ES. These parameter set will be used for the simulation of the in situ experiment conducted at the Mont Terri Rock Laboratory. Currently, a large-scale in situ experiment is performed to study the processes under real conditions in interaction with the potential host rock. Two mini-shafts with a diameter of 1.2 m and a length of 12 m (BSW-A1) (Fig. 11a) and 10 m (BSW-A2) have been drilled. The implementation of four DS segments (Calcigel bentonite) and five ES segments and the installation of measuring sensors have been completed in the BSW-A1. Before implementation, the hydraulic properties of the rock and shaft surface were characterized. A near-field damage zone (EDZ) with a relatively higher permeability around the shaft was measured. The thickness is, however, relatively small according to the measurement (Shao 2022a). Artificial hydration is realized by injecting water from the bottom of the shaft.

A true three-dimensional model is required to account for the anisotropic hydraulic and mechanical properties of Opalinus clay (Fig. 11b). The model includes an EDZ with a thickness of 1 cm (mesh in blue color in Fig. 10b). A saturation state after drilling the shaft was determined with this model (Fig. 11c). It serves as the initial condition for the ongoing hydration process in the in situ sandwich experiment. Predictive modelling of the in situ experiment using the parameter obtained from this study is still ongoing and results will be compared with the field data in several years.

6 Conclusions

To demonstrate the functionality of the Sandwich concept developed by KIT (Nüesch et al. 2002), a series of experiment at different scales (both the MiniSandwich and technical scale in the laboratory as well as a large-scale experiment in situ at the Mont Terri Rock Laboratory, CH) are being performed by the project partner (Emmerich et al. 2019). The simple MiniSandwich tests carried out at the IfG under well-controlled test conditions are very helpful for understanding the processes in the Sandwich sealing system and

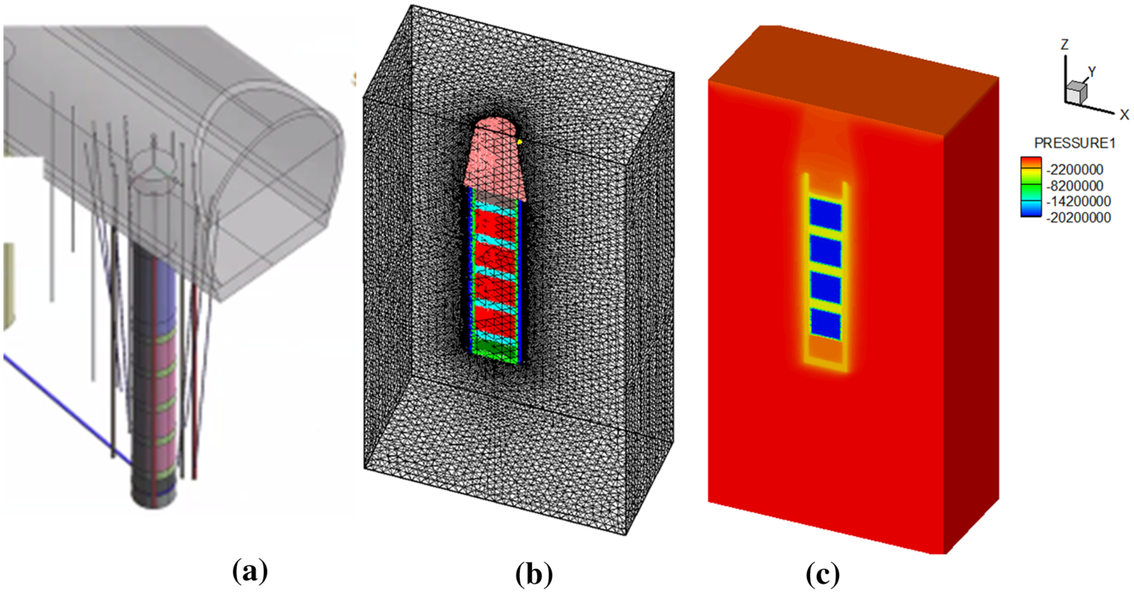

Fig. 11 **a** Layout of the in-situ Sandwich test at the Mont Terri Rock Laboratory, **b** a half model considering anisotropy and EDZ, and **c** calculated desaturated zone before installation of DS and ES in situ

provide all the important information for model calibration and validation as well as a parametrization of the individual components.

To simulate the stress and flow evolution in the MiniSandwich experiments, an axisymmetric 2D model was developed using FE code OGS. The model is based on a fully coupled hydromechanical algorithm taking into account the swelling deformation of DS and deformation-induced permeability changes in DS and ES, in particular the interaction between DS and ES. Two experiments with different dry densities for DS (1.55 g/cm^3 of Calcigel and 1.33 g/cm^3 of Secursol UHP/sand mixture) and the same Pearson injection water were simulated using the same model. With the proposed model, the most important processes and characteristic pattern in this Sandwich sealing system for both measured axial stress and inflow can be captured numerically. Intensive variations of the most important parameters, e.g. permeability/porosity, retention curve, Young ‘s modulus, Poisson’s ratio, swelling pressure, and the empirical permeability-strain-function, were carried out as sensitivity analysis to reduce the parameter uncertainty. The results from the different parameter combination show an improvement in the agreement between the measured and calculated data, but no significant change in the characteristic pattern. The permeability and the maximum swelling stress, which depend on the dry density of the bentonite, are the two key parameters for the system behavior of the sandwich system.

The validated model with the defined parameter set is applied to the design calculation and interpretation of the in situ experiments carried out at the Mont Terri Rock Laboratory.

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Data availability All image and raw data are only available to project partners and are not publicly accessible due to commercial restrictions.

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