



ARBEITSBERICHT NAB 24-27

Gas-related Property Distributions in the
Proposed Host Rock Formations of the
Candidate Siting Region in Northern
Switzerland – Updated Database 2024

October 2024

**Nagra | National Cooperative for the
Disposal of Radioactive Waste**

Hardstrasse 73 | 5430 Wettingen | Switzerland
+41 56 437 11 11 | info@nagra.ch | nagra.ch



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KEYWORDS

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L/ILW, HLW

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Abstract

In Stage 3 of the Sectoral Plan for Deep Geological Repositories in Switzerland (SGT), the three potential siting regions Jura Ost (JO), Nördlich Lägern (NL) and Zürich Nordost (ZNO) were examined in detail. The broadened site-specific database formed the basis for selecting the Haberstal site in the NL siting region for a repository for the disposal of spent fuel and high-level waste from reprocessing (SF/HLW) and low- and intermediate-level waste (L/ILW). Nagra is currently preparing the general licence application for the Haberstal site in the NL siting region. This report summarises and integrates the lines of evidence which have proven beneficial for broadening the existing gas-related database of the host rock (Opalinus Clay) and the confining geological units in the three siting regions. Gas-related properties and thermo-hydro-mechanical (THM) properties of the geological barriers and the engineered barrier system (EBS), such as porosity, intrinsic permeability, relative permeability, capillary pressure, thermal conductivity, and heat capacity, which all provide input for the qualitative assessment of the 13 SGT criteria in the context of the site selection process and for the modelling of gas release related to the performance assessment (PA) and safety assessment (SA), contributing to the safety case for a repository in the NL siting region.

The report provides a brief introduction to the fundamentals of gas transport in porous media. A comprehensive survey of the available field and laboratory data is compiled and documented. Data sources encompass previous site investigation programmes, the latest deep borehole campaign (TBO) in the three siting regions, RD&D activities at the Mont Terri Underground Rock Laboratory (URL) and on other international research platforms (including the EURATOM projects NF-PRO, FORGE and EURAD-GAS). The gas-related databases are interpreted and subjected to model-supported analyses, finally constituting the gas-related reference dataset for the Opalinus Clay, for the confining geological units in the three siting regions and for the EBS.

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List of Acronyms

BC	Boom Clay (potential host rock of the Belgian Radioactive Waste Management Programme)
BET/BJH	Brunauer-Emmett-Teller (BET) surface area analysis and Barrett-Joyner-Halenda (BJH) pore size and volume analysis
BD	«Brauner Dogger» (“Brown Dogger” – clay-rich sequences in the upper confining geological units assessed in SGT Stage 2 as a potential host rock formation in the potential siting regions JO; NL and ZNO)
BIB	Broad ion-beam (imaging)
BSE	Backscattered electron (imaging)
COx	Calovo-Oxfordian (host rock of the French Radioactive Waste Storage Programme)
CRZ	Confinement-providing rock zone
DGR	Deep geological repository
EBS	Engineered barrier system
EDZ	Excavation-damaged zone
EPFL/LMS	Swiss Federal Institute of Technology Lausanne (École Polytechnique Fédérale de Lausanne) / Laboratory of Soil Mechanics (Laboratoire de Mécanique des Sols)
ENSI	Swiss Federal Nuclear Safety Inspectorate (<i>Eidgenössisches Nuklearsicherheitsinspektorat</i>)
EURAD-GAS	European Joint Programme on Radioactive Waste Management – GAS (Mechanistic Understanding of Gas Transport in Clay Materials) work package
EURATOM	European Atomic Energy Community
FDT	Fluid displacement technique (with the Kerdane method)
FIB-nt	Focused ion-beam nanotomography
FORGE	Fate of Repository Gases (EURATOM Project / FP7)
GRS	Germany’s central expert organisation in the field of nuclear safety and radioactive waste management (Gesellschaft für Reaktorforschung)
GTPT	Gas threshold pressure test
HE-E	In-situ Heater Test in VE Microtunnel
HTO	Tritiated water
IP	Invasion percolation
JO	Jura Ost (siting region)
KBA	Limestone bed sequences (<i>Kalkbankabfolgen</i>)
KMA	Calcareous marl sequences (<i>Kalkmergelabfolgen</i>)

L/ILW	Low- and intermediate-level waste
MIP	Mercury intrusion porosimetry (method)
NAB	Nagra Work Report (<i>Nagra Arbeitsbericht</i>)
NEA	Nuclear Energy Act
NFPRO	Understanding and Physical and Numerical Modelling of the Key Processes in the Near-Field and their Coupling for Different Host Rocks and Repository Strategies (EURATOM / FP5)
NTB	Nagra Technical Report
NL	Nördlich Lägern (siting region)
OPA	Opalinus Clay
PA/SA	Performance assessment / safety assessment
PEBS	Long-term Performance of Engineered Barrier Systems
PSD	Pore-size distribution
RD&D	Research, development and demonstration
RVE	Representative volume element
SEM	Scanning electron microscopy
SF/HLW	Spent fuel / high-level waste
SFOE	Swiss Federal Office of Energy
SGT	Sectoral Plan for Deep Geological Repositories (<i>Sachplan geologische Tiefenlager</i>)
STP	Standard temperature and pressure
THM	Thermo-hydro-mechanical
TBO	Deep borehole campaign (<i>Tiefbohrkampagne</i>)
UCS	Unconfined compressive strength
UPC	Universitat Politècnica de Catalunya (Barcelona, Spain)
URL	Underground research laboratory
WRC	Water retention curve
ZNO	Zürich Nordost siting region

1 Introduction

1.1 Background

The procedure for selecting the sites for the deep geological repositories in Switzerland has been specified in the conceptual part of the Sectoral Plan for Deep Geological Repositories (SGT) (SFOE 2008) and consists of three stages. In Stage 3, the three remaining potential siting regions Jura Ost (JO), Nördlich Lägern (NL) and Zürich Nordost (ZNO) were examined in detail and, where necessary, supplementary geological investigations were performed. The broadened site-specific database formed the basis for selecting the NL siting region for a repository with a section for spent fuel and high-level waste (SF/HLW) and a section for low- and intermediate-level waste (L/ILW), respectively, for which the general licence application will be prepared.

This report summarises and integrates the lines of evidence which have proven useful for broadening the existing gas-related database of the host rock and confining geological units. The gas-related properties and thermo-hydro-mechanical (THM) properties of the geological barriers and the engineered barrier system (EBS), such as porosity, intrinsic permeability, relative permeability, capillary pressure, thermal conductivity and heat capacity are input for the qualitative assessment of the 13 criteria specified in SGT in the context of the site selection process and for the modelling of gas release in connection with the performance assessment and safety assessment (PA/SA), contributing to the safety case for a combined repository in the NL siting region.

The report provides a brief introduction in the fundamentals of gas transport in porous media. A comprehensive survey of the available field and laboratory data is compiled and documented. Data sources include previous site investigation programmes, the latest deep borehole campaign (TBO) conducted in the three siting regions, RD&D activities at the Mont Terri Underground Rock Laboratory (URL) and on other international research platforms (including the EURATOM projects NF-PRO, FORGE and EURAD-GAS). The gas-related databases are interpreted and subjected to model-supported analyses, finally constituting the gas-related reference dataset for the Opalinus Clay, the confining geological units in the three siting regions and the EBS.

1.2 Objectives

Spatial distributions of gas-related properties, such as porosity, intrinsic permeability, relative permeability and capillary pressure are a key input for modelling the gas release from deep geological repositories in the proposed siting region and from the different materials used for the EBS. For this, a comprehensive survey of the available field and laboratory data is needed. The integrated interpretation of the raw data requires a traceable methodology. It is the purpose of the present report to:

- Briefly introduce the fundamentals of gas transport in porous media.
- Provide a comprehensive survey of the existing hydrogeological databases needed for the inference of gas-related property distributions of the host rock formation in the proposed siting region and of the EBS components.
- Set out a traceable workflow for an integrated interpretation methodology that provides representative gas transport parameter estimates from the existing mineralogical and hydrogeological database.
- Apply the developed workflow to the available data from the host rock formation to derive conceptual flow models, rock-specific porosity-permeability-entry pressure relationships and, finally, representative estimates of the gas transport parameter distributions and the corresponding parameter uncertainties.

- Provide gas-related reference parameter sets for the host rock formation and EBS components, which can be used as input for modelling gas-release scenarios.
- Compare the results with information from similar rock types investigated in site characterisation programmes for the deep geological disposal of radioactive waste in Europe and in other geoscientific disciplines, such as oil and gas exploration, CO₂ sequestration and the mining industry.

1.3 Geoscientific database – current state of knowledge

The candidate siting regions are situated in the Molasse Basin and the Tabular Jura of Northern Switzerland, respectively. This paragraph gives a brief survey of previous gas-related studies and summarises recent activities initiated in the context of narrowing down potential siting region in Stages 2 and 3 of the SGT.

As part of previous site investigation programmes, Nagra has spent comprehensive efforts in characterising the gas transport behaviour of the investigated host rock formations and EBS components. The main data sources can be linked to the following programmes and research platforms:

- OPA/*Entsorgungsnachweis*: Characterisation of gas-related properties of the Opalinus Clay by laboratory tests and packer tests in the context of demonstrating disposal feasibility (e.g., Nagra 2002 as well as the Schlattingen and TBO boreholes).
- Mont Terri URL: A series of gas-related laboratory and in-situ experiments (Marschall et al. 2005, Croisé et al. 2006).
- EU projects: Laboratory tests and field experiments performed in various URLs in argillaceous formations (NFPRO, FORGE, Boom Clay, COX).
- Complementary desk studies comprising evidence from elsewhere (CO₂, natural gas storage, reservoir engineering, shale gas).

In the context of Stage 2 of the Sectoral Plan, further gas-related studies have been initiated to complement the existing gas-related database for the candidate host rock formations (Nagra 2010, Marschall et al. 2013, SHARC Consortium 2013). Furthermore, Nagra participated in various drilling and logging campaigns in the context of geothermal energy exploration in Northern Switzerland. Core samples from the different host rock formations were recovered and subjected to detailed mineralogical and geotechnical laboratory analyses. In several boreholes, it was possible to perform packer test campaigns in candidate host rock formations. Tab. 1-1 gives an overview of recent investigations that are relevant to the present report.

Tab. 1-1: Reference reports of particular relevance for the survey of gas transport parameters of the candidate host rock formations

Topic	Report
<i>Hydraulic and physical rock properties</i>	
Beauheim (2013): Hydraulic conductivity and head distributions in the host rock formations of the proposed siting regions. Nagra Arbeitsbericht	NAB 13-13
Sarout et al. (2012): Laboratory Characterisation of Cores (Geothermal Well Schlattingen SLA-1, Switzerland): Petrophysics and rock mechanics / physics. Nagra Arbeitsbericht.	NAB 12-47
Gesteinslabor (2012): Bohrung Gösgen KB-5A – Felsmechanische Untersuchungen an Kernen der Effinger Schichten. Nagra Arbeitsbericht.	NAB 11-08
Mazurek (2011): Aufbau und Auswertung der Gesteinsparameter-Datenbank für Opalinuston, den 'Braunen Dogger', Effinger Schichten und Mergel-Formationen des Helvetikums. Nagra Arbeitsbericht.	NAB 11-20
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Tab. 1-1: Cont.

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<i>EURAD</i>	
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Levasseur et al. (2024): State of the Art on Gas Transport in Clayey Materials – Update 2023. Deliverable D6.2 of the HORIZON 2020 project EURAD, Work Package Gas. EC Grant agreement no: 847593.	EURAD D6.2
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Marschall et al. (2024): Final Report on gasinduced impacts comprising the experimental results of Subtasks T 3.1 and 3.2 – contribution to the thematic report on barrier integrity / Part 1. Deliverable D6.8 of the HORIZON 2020 project EURAD. EC Grant agreement no: 847593.	EURAD D6.8

1.4 Report outline

Chapter 1 describes the scope and background of this report within the context of Stage 3 of the SGT and details the objectives of the presented gas-related analyses. A survey of relevant literature and a brief report outline are given.

Chapter 2 presents the fundamentals of gas transport in porous media, comprising gas transport mechanisms, parametric models of two-phase flow and an overview of important coupled processes.

The integrated interpretation of the gas-related laboratory and field data from the host rock formation (Opalinus Clay) and the confining geological units (clay-rich and calcareous sequences), is described in Chapter 3. Gas-related reference parameters are given in tabular form for the host rock and the confining units, respectively.

Chapter 4 provides the gas-related properties of the EBS components which include: bentonite, sand/bentonite mixtures and concrete/mortar.

Chapter 5 summarises the current state of knowledge on the gas-related properties of the selected host rock formation and confining units in the proposed siting region with a view to preparing the general licence application in Stage 3 of the SGT.

2 Gas transport in clay-rich host rocks – fundamental principles

2.1 Rationale

The release of the gases produced in the backfilled disposal systems of the repository can occur by a variety of transport mechanisms. Gases will dissolve in the porewater and eventually, when the solubility limit has been exceeded, a separate phase will form, initiating a two-phase flow. At elevated gas pressures, the porous medium (host rock and backfill material, respectively) can undergo mechanical deformation, which can significantly impact its flow and transport properties.

The prevailing gas transport mechanisms are controlled by the hydrodynamic properties of the fluids and by the environmental conditions, such as in-situ pore pressure, rock stress and water saturation in the porous medium. The microstructural and macroscopic characteristics of the porous medium are of special importance for the hydrodynamic properties, including the pore-size distribution, pore connectivity, spatial variability of the porosity and the mineralogical composition of the solid phase (wettability). It is the purpose of this chapter to provide a systematic overview of the main gas transport processes, the gas-related parameters and the coupled processes which can be associated with the transport of the gas through the host rock formation (Opalinus Clay) and overlying confining geological units (clay-rich and calcareous sequences). Furthermore, the conceptual frameworks are presented for modelling gas transport processes in porous media. The chapter is structured as follows:

- Gas transport mechanisms in the porous rock matrix: The relevant gas transport mechanisms are specified, their characteristic features are discussed and the corresponding parameterisation of transport mechanisms is given (Section 2.2).
- Modelling of gas transport processes in heterogeneous media (Section 2.3).

2.2 Gas transport mechanisms: phenomena and conceptual models

Gas transport through low-permeability rock formations is controlled not only by the hydraulic and mechanical properties of the rock mass (intrinsic permeability, porosity, rock strength), but also by the gas pressure at the location of gas entry and the hydromechanical state of the rock (i.e., water saturation, porewater pressure, stress state). Phenomenological considerations suggest the following subdivision of the basic transport mechanisms (Marschall et al. 2005; Fig. 2-1):

- advective-diffusive transport of gas dissolved in the porewater;
- visco-capillary two-phase flow;
- dilatancy-controlled gas flow;
- gas transport along macroscopic tensile fractures (hydro- and gas-fracturing).

The phenomenological description of flow and transport processes is related to the microstructural conceptualisation of the porous medium. In ultra-low permeability rock such as the Opalinus Clay, a network of connected pores in the micro- to nanometre range defines the space, where flow of immiscible fluids can happen. Assuming that the skeleton of the solid rock matrix is subjected to elastic deformations only – in other words, the void volume of the pore network remains essentially constant – the flow of liquids and gases in the porous network can be described by well-known hydrodynamic approaches, such as (multiphase) flow in equivalent porous media and flow in channel/fracture networks, respectively.

The degree of complexity increases when two-phase flow processes occur in a deformable porous medium (solid phase). In this case, the relevant state variables (i.e., displacements, forces) of all three phases are interdependent (i.e., coupled) and, as a consequence, the void volume of the pore network is no longer constant but is controlled by the state of deformation of the solid skeleton. In fracture mechanics terminology (e.g., Gross & Seelig 2007), irreversible deformation of the solid skeleton can be associated with ductile fracturing (subcritical crack growth) or brittle fracturing (supercritical crack growth). Ductile fracturing is characterised by extensive plastic deformation before fracture initiation and slow fracture propagation, associated with absorption of a large amount of energy. In contrast, brittle fracturing is not associated with measurable plastic deformation before fracture initiation. The fracture propagates smoothly along the stress gradient and creates extended tensile cracks.

The different gas transport mechanisms are discussed in the following sections. A key issue in the quantitative description of two-phase flow processes is addressed in Section 2.3, which deals with the definition of a representative elementary volume of combined gas/water flow and with the upscaling of two-phase flow parameters.

It is worth mentioning that different terms can be found in the geoscientific literature to describe gas transport processes. The term “capillary failure” is often used in the oil and gas industry to describe the two-phase flow regime in cap rocks (e.g., Clayton & Hay 1994). “Membrane seal failure” describes gas transport through the pre-existing pore system of the cap rock (i.e., advection/diffusion of dissolved gas and two-phase flow), whereas “hydraulic seal failure” is used to describe gas leakage due to hydro-mechanical processes in the seal (microfracturing, reopening of existing faults, hydro/gas fracturing). A comprehensive literature study on gas storage and gas transport phenomena is given in Evans & West (2008).

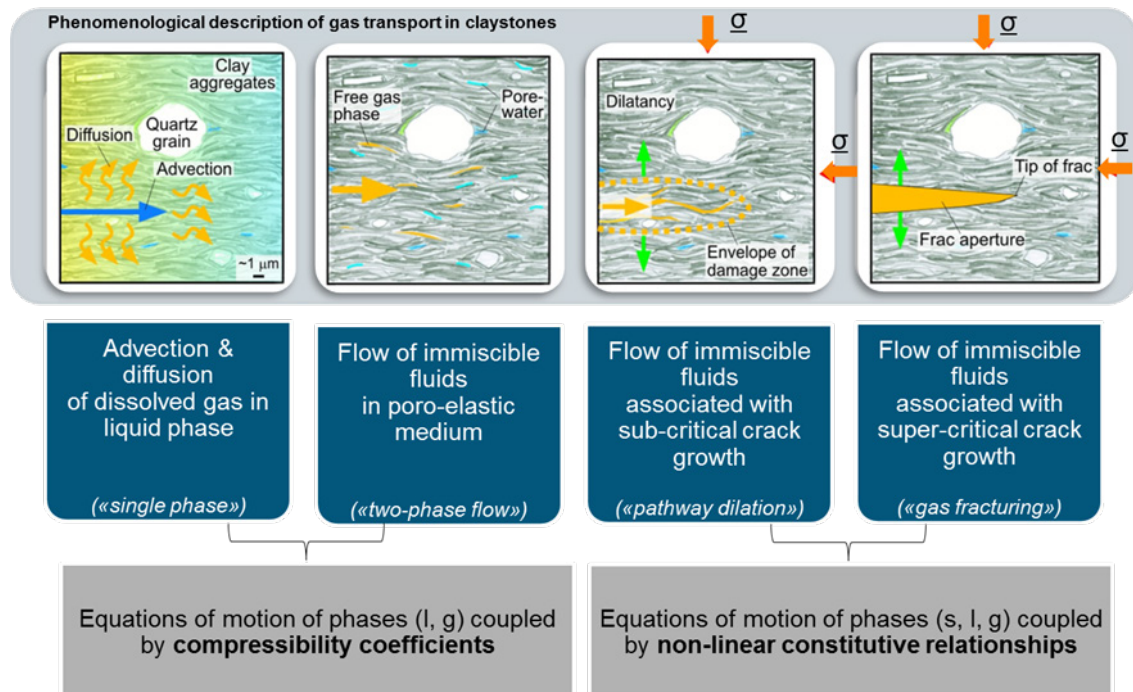


Fig. 2-1: Classification and analysis of gas transport processes in ultra-low permeability rock such as the Opalinus Clay

2.2.1 Transport of gas dissolved in the porewater

Advective and diffusive transport of gas dissolved in porewater is characterised by three fundamental laws (Helmig 1997):

- Darcy's law describes advective groundwater flow under the impact of pressure and gravitational forces.
- Fick's law represents the diffusion of dissolved gas due to concentration gradients in the porewater.
- Henry's law describes the solubility of gas in porewater.

In this context, sorption of gas on clay has been identified as a possible retardation mechanism for dissolved gas transport or gas phase transport (Didier et al. 2012). This mechanism is not considered in the present appraisal, because the sorption potential of the clay minerals decreases with increasing saturation of the rock. For the release of gases through the host rock formation, this retardation process is expected to be of very limited relevance.

Darcy's law represents the general basis for quantitative descriptions of groundwater flow. It denotes the linear correlation between the specific discharge (Darcy velocity) through a representative elementary volume and the hydraulic gradient. The proportionality constant for the relationship is provided by the hydraulic conductivity, K . Darcy's law is applicable only within certain limitations. For geomaterials with ultra-low permeability, such as the Opalinus Clay and bentonite, deviations from the linear flow law may be expected for low hydraulic gradients. The small pore radii cause electro-molecular rock-water interactions to gain significance in comparison to the viscous fluid properties, i.e. friction. In response, the formation water no longer behaves like a Newtonian fluid when exposed to a low hydraulic gradient. A comprehensive discussion of possible causes for non-linear porewater flow in clay-rich materials is found in Horseman et al. (1996). In empirical terms, this situation can be accounted for by introducing a hydraulic threshold gradient, (e.g., Bear 1972, Marsily 1986). For the Opalinus Clay, the threshold gradient necessary to establish Darcy flow was assessed by laboratory and in-situ experiments; the investigations indicated that Darcy's law holds for hydraulic gradients > 10 m/m (Marschall et al. 2005).

Diffusion is a process induced by the random thermal motion of molecules and ions. Diffusion in a porous medium in its simplest form can be described by Fick's law (Domenico & Schwartz 1990):

$$J = -D_d \text{grad}(C) \quad (2-1)$$

with J being the diffusional flux ($\text{M/L}^2\text{T}$); D_d the effective diffusion coefficient (L^2/T) and C the concentration (M/L^3) of a species.

In this equation, the flux of each species is related to the concentration gradient by a diffusion coefficient that is specific to that species. The value of the diffusion coefficient of a species in water depends on the type of species, the temperature and pressure and its interaction with other species (Felmy & Weare 1991). Diffusion coefficients for up to 30 species in a wide temperature and pressure range are given in Oelkers & Helgeson (1988).

Tab. 2-1 gives the diffusion coefficients and solubility in free water for a selection of gases, which are relevant for the assessment of gas release.

In the case of diffusion in a porous medium, the diffusion rate is further defined by the structure and the properties of the porous medium such as the effective porosity, describing the total pore space available for the diffusion of the species, and the tortuosity, accounting for the pore space geometry. Among various definitions, one of the most cited is that of Greenkorn & Kessler (1972) expressing D_d as a function of porosity and tortuosity (Greenkorn & Kessler 1972):

$$D_d = \frac{\phi \cdot d_w}{\left(\frac{L_e}{L} \right)} \quad (2-2)$$

In comparison, Grathwohl (1998) and Jacops et al. (2017a) defined a geometric factor G as the ratio between tortuosity τ and constrictivity δ : $G = \tau/\delta$, where the constrictivity takes into account the reduction in the effective diffusion coefficient due to a drag by the pore wall and depends on the ratio of the solute diameter and the pore diameter. The effective diffusion coefficient is then given by:

$$D_d = \frac{\phi d_w}{G} \quad (2-3)$$

In the case of large pores, the constrictivity is equals to one, and becomes much smaller than one if the solute diameter has the same order of magnitude as the pore diameter.

Analogous to the electrical conductivity of water-saturated rocks, the diffusion coefficient in free water and the effective diffusion coefficient can be used to define a “formation factor”, F , defined as:

$$F = \frac{G}{\phi_d} = \frac{d_w}{D_d} \quad (2-4)$$

In general, two transport parameters can be obtained from diffusion experiments as described in Jacops et al. (2017b): the apparent diffusion coefficient D_{app} [m^2/s] and the capacity factor ϕR , being the product of the accessible porosity ϕ (dimensionless) and the retardation factor R (dimensionless), which accounts for retention of the diffusing species by chemo-physical interactions with the solid phase, e.g., gas sorption processes.

From these two basic parameters, the effective diffusion coefficient D_d is calculated as:

$$D_d = \phi \cdot R \cdot D_{app} \quad (2-5)$$

Assuming $R=1$ and $\phi \cdot R$ is constantly equal to ϕ_{tot} , the value for D_{app} is fitted to the experimental data, where the porosity is calculated from the water content of each sample.

Gas dissolution and exsolution can transfer significant quantities of mass between the gaseous phase and the porewater in a porous medium.

According to Henry's law, the partial pressure of an ideal gas in the gaseous phase is proportional to the concentration of the gas in the aqueous phase (Domenico & Schwartz 1990):

$$K_H = \frac{(gas)_{aq}}{P_{gas}} \quad (2-6)$$

where K_H is the Henry's law constant (mol Pa^{-1}), P_{gas} is the partial pressure of the gas in the gaseous phase (Pa) and $(\text{gas})_{\text{aq}}$ is the molar concentration of the gas in solution. Tab. 2-1 provides the solubilities of various gases in water.

This law is only valid for ideal gases and highly dilute porewaters. In the case of real gases, fugacity should be taken into account instead of the partial pressure. Fugacity is a function of the temperature, the pressure and the composition of the gaseous phase. Equally, in the case of more realistic porewater compositions, activities should be used instead of concentrations. Activities are influenced by the pressure, the temperature and the composition of the solution and are significantly lower than the equivalent concentrations in those cases where porewaters consist of concentrated brines at higher temperatures and pressures (Kervévan et al. 2005).

The transport of dissolved gas occurs even at low (total) gas pressures; the pressure-dependent dissolution of gas in porewater and the increased groundwater flux cause the specific flux of the dissolved gas to increase with an increase in the gas pressure. The low hydraulic conductivity of argillaceous rock significantly restricts the efficiency of this transport mechanism. Thus, scoping calculations were conducted as part of the SF/HLW disposal programme, indicating that the gas transport capacity of diffusion and advection (of dissolved gases) is several orders of magnitudes below that of the transport capacity of the two-phase flow (Nagra 2004). Nevertheless, the general importance of diffusion and advection as slow background processes in all types of cap rock formations is beyond question and has been addressed in the context of many hydrocarbon exploration and reservoir engineering studies (Clayton & Hay 1994, Krooss et al. 1992, Schlömer & Krooss 1997).

Tab. 2-1: Solubilities and diffusion coefficients of a selection of gases in water at standard conditions (25 °C, 1 atm)

(From Lide 2000).

Gas	Formula	Solubility (25 °C, 1 atm) in mg L^{-1}	Diffusion (25 °C) $\times 10^{-9} \text{ m}^2 \text{ s}^{-1}$
Hydrogen	H_2	1.58	5.11
Helium	He	1.56	7.28
Oxygen	O_2	40.76	2.42
Nitrogen	N_2	18.41	2.00
Carbon dioxide	CO_2	1,503.52	1.91
Methane	CH_4	22.74	1.84

The free-water diffusion coefficient D_0 for dissolved gases is typically related to the kinetic diameter of the gas molecules as shown in Fig. 2-2 and can be fitted using an exponential or power law function.

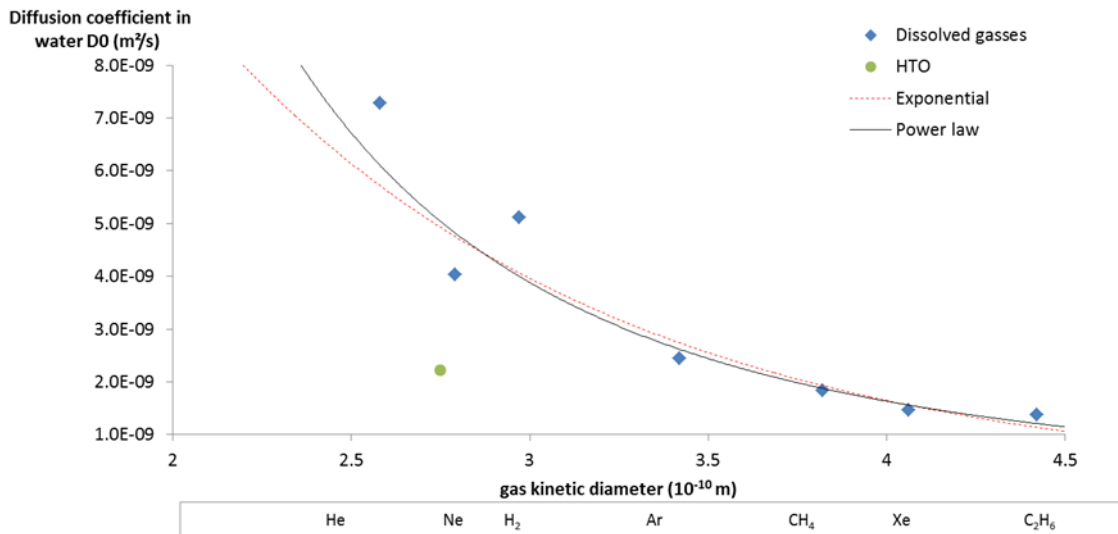


Fig. 2-2: Relation between the diffusion coefficient D_0 in free water and the kinetic diameter for dissolved gases with an exponential fit and a power law fit

He: helium; Ne: neon; H₂: hydrogen; Ar: argon; CH₄: methane; Xe: xenon; C₂H₆: ethane (from Boudreau 1997). The tritiated water (HTO) value is not included in the fit and given only for comparison with dissolved gases (from Levasseur et al. 2021).

Jacops et al. (2017b) and Jacops et al. (2020) integrated diffusion experiments, petrophysical analyses and petrographical studies to characterise the transport properties of different clay host rocks (Boom Clay, Callovo-Oxfordian, Opalinus Clay and bentonite), highlighting the complex relationships between porous medium characteristics, gas molecule size and transport parameters.

As described above, the measured diffusion coefficients represent the apparent diffusion coefficients (D_{app}) from which the effective diffusion coefficients can be calculated using Equ. 2-5. Since diffusion coefficients are specific to the solute type, the transport parameters related to the different materials are an important input parameter, which is related to the tortuosity and/or constrictivity (e.g., geometry factor G in Eq. 2-3).

Fig. 2-3 shows the effective diffusion coefficients of dissolved gases as a function of the kinetic diameter indicating a decrease with increasing kinetic diameter similar to that of the free-water diffusion coefficient but as much as two orders of magnitude below that of the different clays.

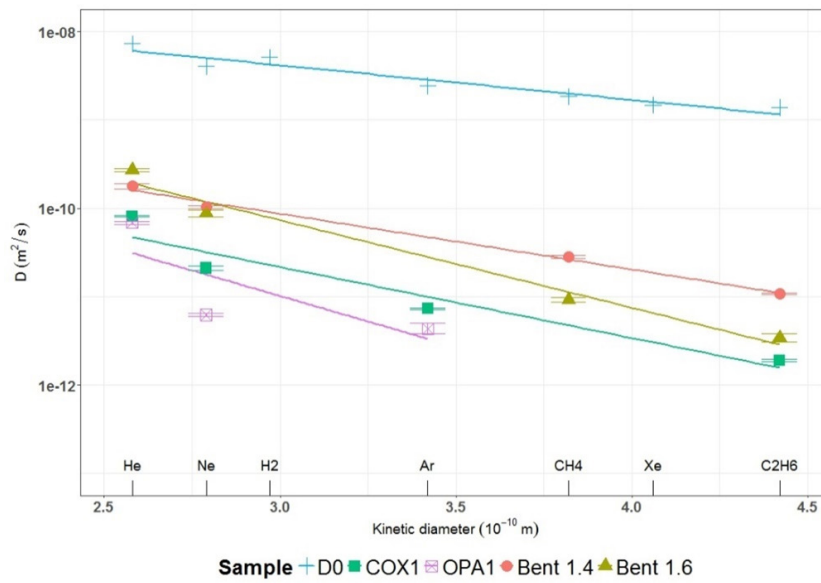


Fig. 2-3: Effective diffusion coefficients for dissolved gases in Callovo-Oxfordian claystone, Opalinus Clay and bentonite, fitted with Eq. 2-5

The diffusion coefficient D is either the diffusion coefficient D_0 in pure water or the effective diffusion coefficient D_p , in a porous medium (Jacops et al. 2017b).

Based on the measured diffusion coefficients and the measured porosity, the geometric factor can be calculated (Eq. 2-3). For Callovo-Oxfordian claystone, the Opalinus Clay and bentonite, the geometric factor is not a constant value but clearly increases with the size of the diffusing molecule (Fig. 2-4).

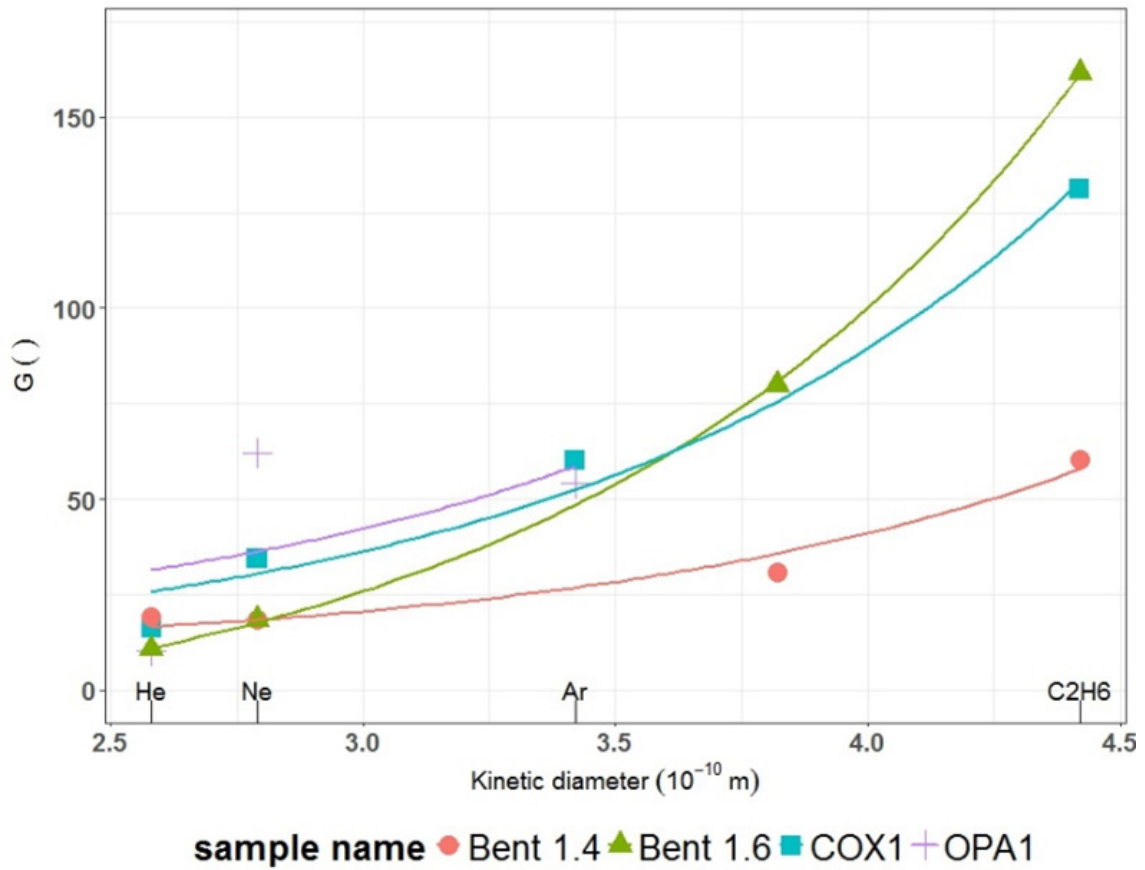


Fig. 2-4: Evolution of the geometric factor with the size of the diffusing molecule for Callovo-Oxfordian claystone (COx), Opalinus Clay (OPA) and bentonite (Bent)

From Jacops et al. (2017b).

The diffusion coefficient for a two-phase system with porosity ϕ is defined as Pruess et al. (1999):

$$D_{\beta}^{\kappa} = \phi \cdot \tau_0 \cdot \tau_{\beta} \cdot d_{\beta}^{\kappa} \quad (2-7)$$

where d_{β}^{κ} is the molecular diffusion coefficient for component κ in phase β , $\tau_0 \tau_{\beta}$ is the tortuosity which includes a porous medium-dependent factor τ_0 and a coefficient that depends on phase saturation S_{β} , $\tau_{\beta} = \tau_{\beta}(S_{\beta})$. The diffusion coefficients for gases depend on pressure and temperature, as defined in Vargaftik (1975) and Walker et al. (1981). The saturation dependence of tortuosity can be described as functional relationships, such as that given by Millington & Quirk (1961):

$$\tau = \phi^{1/3} S_{\beta}^{10/3} \quad (2-8)$$

2.2.2 Visco-capillary two-phase flow

Terminology and phenomenological aspects

Flow of immiscible fluids in porous media – often denoted as two-phase flow when the fluids are water and gas – has been the subject of extensive research in various disciplines of science and engineering, such as the oil and gas industry, CO₂ sequestration and environmental engineering. In its conventional form, visco-capillary two-phase flow is described as a transport process whereby porewater in the pore volume of a rock formation is displaced by gas under the influence of viscous and capillary forces (e.g., Bear 1972). This process is often called drainage, because the non-wetting fluid (gas) displaces a wetting fluid (porewater, “defending” fluid). The propagation of the gas front is controlled by the complex interaction of viscous forces, capillary forces and gravity. Many references of laboratory-scale experiments are found in the literature, with the aim to analyse and classify the governing processes of immiscible fluid flow in porous media (see e.g., Lenormand et al. 1988, Méheust et al. 2002, Glass et al. 2001, Neuweiler et al. 2004, Marschall & Lunati 2006).

Lenormand et al. (1988) conducted two-phase flow experiments for a wide range of capillary numbers C_a and viscosity ratios M (Fig. 2-5):

$$C_a = \frac{\text{viscous forces}}{\text{capillary forces}} = \frac{\mu_{wf} \cdot v_f}{\sigma_{wf, nwf}}$$

$$M = \frac{\mu_{invading}}{\mu_{defending}} = \frac{\mu_{nwf}}{\mu_{wf}} \text{ or } \frac{\mu_{wf}}{\mu_{nwf}} \text{ (instable or stable displacement)}$$
(2-9)

where μ_{wf} and μ_{nwf} represent the viscosities of the wetting and non-wetting fluid, v_f is the characteristic (Darcy) velocity in the medium and $\sigma_{wf, nwf}$ is the surface tension between the two fluids.

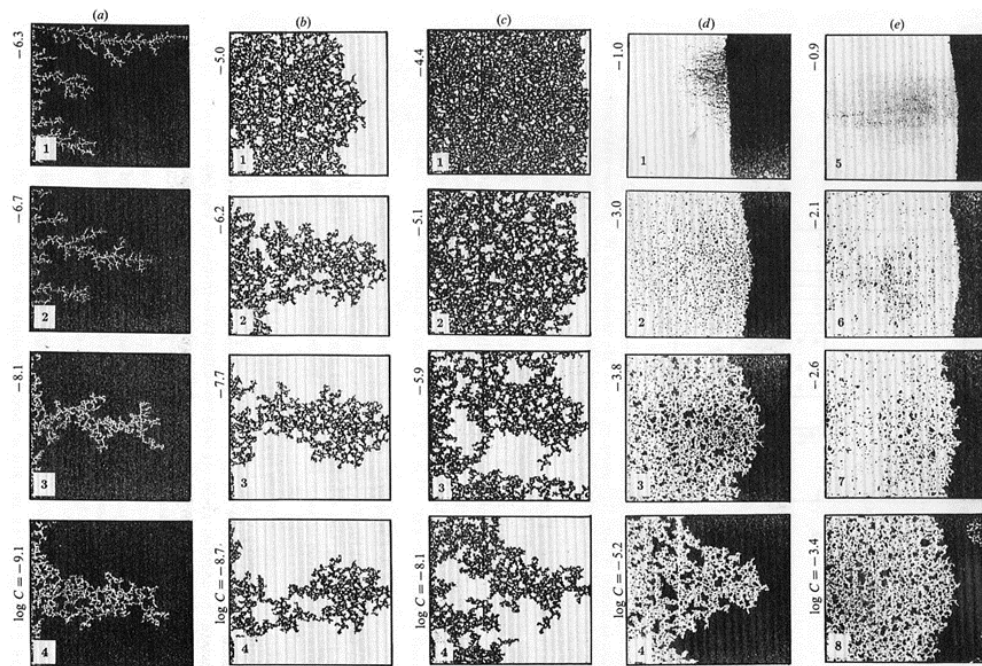


Fig. 2-5: Immiscible displacement in porous media (from Lenormand et al. 1988)

(a) Air displacing a viscous oil; (b, c) mercury displacing hexane; (d, e) glucose displacing oil at different Ca and $\log M$.

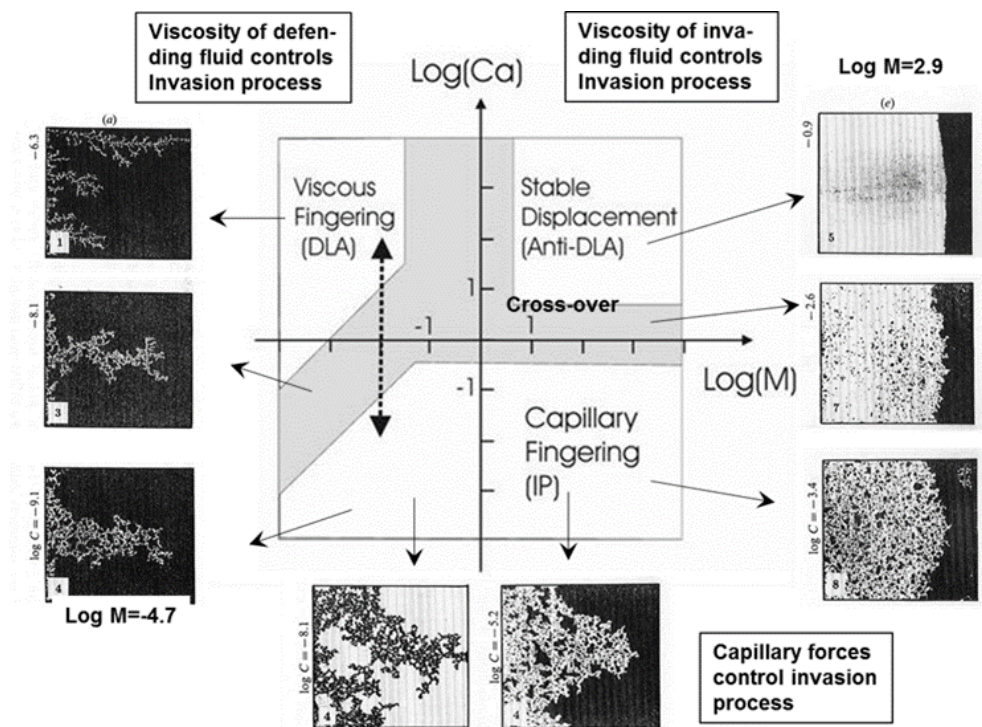


Fig. 2-6: Schematic representation of the three major flow regimes in the Ca - M -space from Lenormand et al. (1988): viscous fingering, capillary fingering and stable displacement

Lenormand et al. (1988) identified three major flow regimes in the C_a - M -space, which they coined viscous fingering, capillary fingering and stable displacement (Fig. 2-6). The regime of stable displacement applies in the special case where the invading fluid has a higher viscosity than the defending fluid, e.g., water imbibition in a gas-filled porous medium (relevant for resaturation processes in the repository near-field). Viscous and capillary fingering are associated with instable displacement of a wetting fluid by the non-wetting fluid, giving rise to phenomena such as migration, fragmentation and coalescence of the non-wetting fluid (Wagner et al. 1997). When a gas front invades the initially saturated matrix of a low-permeability host rock, capillary fingering can be assumed to be the prevailing regime ($\log M \approx -2$; $\log C_a < -10$).

Basic laws of fluid flow

The aforementioned phenomenological studies reveal that flow and transport of liquids and gases are controlled by the microscopic structure of the porous medium. For the following considerations, it is assumed that any type of pore network can be represented by basal elements with pipe-like (channel networks) or planar (fracture networks) shapes.

Laminar flow of an incompressible fluid in a cylindrical pipe is described in fluid mechanics by the Hagen–Poiseuille equation:

$$q = F \cdot k \cdot \nabla P = \frac{\pi \cdot r^4}{8 \cdot \mu} \cdot \nabla P \quad (2-10)$$

where r is the pipe radius, F is the cross-sectional area, k is the intrinsic permeability, ρ and μ are the density and viscosity of the fluid and P is the fluid pressure. Similarly, flow between two parallel plates can be expressed in terms of the cubic law:

$$q = T \cdot w \cdot \nabla P = \frac{a_h^3}{12 \cdot \mu} \cdot w \cdot \nabla P \quad (2-11)$$

where T is the fracture transmissivity, a_h represents the distance between the two parallel plates and w is the trace length.

When gas enters an initially water-saturated capillary tube, the Young-Laplace equation gives the relationship between the gas entry pressure (capillary threshold pressure) and the pore radius:

$$P_{ae} = \frac{2 \cdot \sigma_{gw}}{r} \cdot \cos \alpha \quad (2-12a)$$

where P_{ae} is the gas entry pressure, σ_{gw} is the surface tension gas/water (ca. 0.073 N m^{-1} at 20°C), r represents the radius of the capillary tube and α is the wetting angle.

The corresponding Eq. 2-12b holds for the parallel plates, when the pore radius is exchanged by half the width a_h of the parallel plates:

$$P_{ae} = \frac{4 \cdot \sigma_{gw}}{a_h} \cdot \cos \alpha \quad (2-12b)$$

Drawing on the aforementioned flow laws, pore scale modelling approaches are capable of describing multiphase flow processes in complex channel/fracture networks (see Section 2.3). Nevertheless, it is a great challenge to characterise the porescale variability of low-permeability rocks such as the Opalinus Clay in sufficient detail, as required for an adequate numerical simulation of gas transport processes on the macroscopic scale. Therefore, alternative approaches have been developed. If the length scale of the considered flow processes is much larger than the scale of the microscopic variability, the flow may no longer depend on the details of the small-scale properties. It can then be described as a flow process in an equivalent homogeneous medium, where its medium properties capture the impact of the heterogeneities in an averaged sense. In the classical mixing theory of continuum mechanics of fluids (e.g., Coussy 2004), the three phases (solid, wetting fluid, non-wetting fluid) are assumed to superimpose each other at a given location of the porous medium, and the fluxes of the individual phases are described by the multiphase version of Darcy's law (linear fluid dissipation):

$$v_\beta = -k \cdot \frac{k_{r\beta} \rho_\beta}{\mu_\beta} \cdot (\nabla P_\beta - \rho_\beta \cdot g) \quad (2-13)$$

where v_β is the Darcy velocity (volume flux) in phase β , k is the intrinsic permeability, $k_{r\beta}$ is relative permeability to phase β , μ_β is viscosity, and $P_\beta = P + P_{c\beta}$ is the fluid pressure in phase β , P the pressure of a reference phase (in the TOUGH2 code usually the gas phase, Pruess et al. (1999) and the capillary pressure $P_{c\beta}$. The coefficient g is gravitational acceleration.

Here, it is assumed that the rock mass behaves like an elastic medium, characterised by porosity and rock compressibility. The controlling factor for the two-phase flow characteristics of a porous medium is the gas entry pressure p_{ae} , also known as the capillary threshold pressure, which represents the difference between gas pressure and water pressure needed to displace the porewater from the initially fully saturated medium.

Once the gas entry pressure has been exceeded, the gas mobility is controlled mostly by the intrinsic permeability k of the formation, the permeability-saturation relationships (relative permeability) and the relationship between the capillary pressure and water saturation (suction or water retention curve). The functional dependency between the pore space saturation and the relative permeability or the capillary pressure is commonly described with parametric models, such as that by van Genuchten (1980), gives the functional relationship between water saturation and capillary pressure as:

$$P_c = P_g - P_w = \frac{1}{\alpha} \cdot (S_e^{\frac{n}{n-1}} - 1)^{\frac{1}{n}} \quad (2-14)$$

with

$$S_e = \frac{S_w - S_{wr}}{1 - S_{wr}}$$

or, alternatively:

$$S_e = [1 + (P_c/P_o)^n]^{-(1-1/n)} \quad (2-15)$$

where P_c , P_g and P_w represent the capillary pressure, gas pressure and water pressure, respectively. $1/\alpha$, the inverse of van Genuchten's α parameter, is known as the capillary strength parameter P_o or apparent gas entry pressure, and n is the shape factor (pore-size distribution index). The degree of saturation S_w is the volume of porewater per volume of pores.

A related model which originated in reservoir engineering literature is the Brooks-Corey model, where the capillary pressure is given as a function of saturation:

$$P_c = P_d \cdot S_{e'}^{-1/\lambda} \quad (2-16a)$$

with:

$$S_{e'} = \frac{S_w - S_{wr}}{1 - S_{wr}}$$

where P_d is the capillary air-entry pressure, and the shape parameter λ is related to that in the van Genuchten model by:

$$\lambda = n - 1 \quad (2-16b)$$

As indicated in Eq. (2-12), the capillary pressure depends on the surface tension of water, which is a function of temperature. This means that, for different temperatures, the effective capillary pressure can be specified by:

$$P'_c = P_c \cdot \frac{\sigma(t)}{\sigma_0} \quad (2-17)$$

In the multiphase flow code TOUGH2 (Pruess et al. 1999), the functional relationship is given as:

$$P'_c = P_c \cdot \left[\frac{\sigma}{\sigma_0} - 0.0017 \cdot (T - T_0) \right] \quad (2-18)$$

where σ is the surface tension at a given temperature T and σ_0 is the surface tension at a reference temperature T_0 .

The relative gas/water permeabilities $k_{r,g}$ and $k_{r,w}$ of the Opalinus Clay can be derived by integrating the capillary pressure curve following the approach by Mualem (1976):

$$k_{r,g} = (1 - S_e)^\varepsilon \cdot (1 - S_e^{\frac{n}{1-n}})^{2(1-1/n)} \quad (2-19)$$

$$k_{r,w} = S_e^\gamma \cdot \left[1 - (1 - S_e^{\frac{n}{1-n}})^{\frac{n-1}{n}} \right]^2 \quad (2-20)$$

with

$$S_e = \frac{S_w - S_{wr}}{1 - S_{wr}}$$

where ε and γ are empirical shape factors, describing the pore connectivity of the media which are typically set to $\varepsilon = 1/2$ and $\gamma = 1/3$ (Luckner et al. 1989). With the Mualem approach, relative permeability and capillary pressure are theoretically linked by the shape factor n , which occurs in both equations and is typically determined by the water retention curve.

In the Brooks-Corey model, the relative permeabilities are defined as:

$$k_{r,g} = (1 - S_e)^2 \cdot (1 - S_e^{\frac{2+\lambda}{\lambda}})^{\frac{2+\lambda}{\lambda}} \quad (2-21)$$

$$k_{r,w} = S_e^{\frac{2+3\lambda}{\lambda}} \quad (2-22)$$

with

$$S_e = \frac{S_w - S_{wr}}{1 - S_{gr} - S_{wr}}$$

An excellent review of the spectrum-relative permeability models in multiphase flow analysis is given in Honarpour et al. (1986).

Enhancement (or reduction) of the gas mobility, as postulated in Croisé et al. (2006) for the interpretation of in-situ gas injection tests at the Mont Terri Underground Rock Laboratory, can be taken into account by introducing a multiplication factor f_g in the relative permeability equation, for example for the van Genuchten model, as follows:

$$k_{r,g} = f_g (1 - S_e)^\varepsilon \cdot (1 - S_e^{\frac{n}{1-n}})^{2(1-1/n)} \quad (2-23)$$

In this study, the gas enhancement factor $f_g = 1$ was used for all two-phase flow simulations.

Alternatively, the enhanced gas mobility is described by the Grant model (Grant 1977), where the relative permeability of the gas phase is given as:

$$k_{r,g} = 1 - k_{r,l} \quad (2-24)$$

where the gas and liquid phases tend to move independently of each other. This is typical for fracture-porous rocks where liquids tend to migrate primarily through the matrix due to higher capillary pressures, and gas migrates through the higher-permeable fractures characterised by lower capillary pressures.

A distinct hysteresis is often seen in the capillary pressure relationship, depending on the saturation path, i.e., whether the relationship corresponds to a saturation or desaturation of the porous medium. During the saturation process, the porosity of the medium cannot be saturated completely (residual gas saturation S_{gr}), because part of the pore space is poorly connected. On the other hand, assuming an initially fully saturated medium, a critical gas saturation has to be exceeded before gas starts to form a continuous phase with a gas permeability > 0 (e.g., Dury et al. 1999). In the context of this study, due to the limited experimental database, no distinction is made between residual and critical gas saturation.

The dependency of capillary pressure on the history of flow is known as the aforementioned capillary pressure hysteresis. The dependence of capillary pressure (and of the relative permeability relationship) on the rate of change of saturation is termed in literature as “dynamic effect” or “non-equilibrium effect”. A multitude of references on the dynamic effect are found in the literature (Barenblatt et al. 1990, Hassanizadeh et al. 2002, Silin & Patzek 2004, Schembre & Kovscek 2006, Juanes et al. 2006), however, the interpretation of the effect is controversial. Thus, Hassanizadeh et al. (2002) explain the non-equilibrium phenomenon as a characteristic feature in the context of new macroscopic theories of multiphase flow (Hassanizadeh & Gray 1990), whereas Bourgeat & Panfilov (1998) interpret it as consequence of the upscaling of two-phase flow parameters. In the present report, the dynamic effect is not considered due to the lack of experimental evidence for ultra-low permeability rock, such as Opalinus Clay.

Juanes et al. (2006) investigate hysteresis effects in the relative relationship between permeability and saturation as part of a modelling study on CO₂ sequestration. Drawing on experimental evidence, the authors demonstrate by means of an analysis of pore-scale processes that relative permeabilities are not single functions of fluid saturations (“dynamic effects”) and that they display strong hysteresis effects. Permeability hysteresis could be of great importance for the gas release from deep geological repositories for radioactive waste, because the rock zone around the underground structures is desaturated during the operational phase of the repository. After repository closure, trapped gas in the vicinity of the backfilled tunnels could lower the gas entry pressure of the rock and thus increase its gas transport capacity in the early post-closure period.

Dilatancy-controlled gas flow

Dilatancy-controlled gas flow (or “pathway dilation”; terminology after Horseman et al. (1996)) is a transport mechanism of special importance for argillaceous media with low tensile strength. Clay-rich rock cannot withstand long-term gas pressures with a magnitude greater than the minimum principal stress acting on the rock mass. Due to the expected microscale variability of the geomechanical rock properties, it is even plausible that microfractures will form before yielding (ductile fracturing). Ductile fractures propagate slowly, the fracture surface is rough and the damage zone around the fracture tip grows with increasing distance to the locus of initiation (e.g., Gross & Seelig 2007). The process of gas-driven microfracturing leads to an increase of the void space, which is accompanied by a detectable increase in intrinsic permeability and a change

in the capillary pressure-saturation relationship. In the terminology of multiphase flow concepts, gas flow is still controlled by visco-capillary forces (phase interaction between wetting and non-wetting fluid) – the main difference with respect to conventional two-phase flow is that the transport properties of the solid phase (rock permeability, relative permeability, capillary pressure relationship) can no longer be viewed as invariants since they depend on the state of deformation of the rock.

Olivella & Alonso (2008) developed a hybrid formulation of pathway dilation, expressing the effective permeability of the rock as the superposition of an intrinsic matrix permeability and a stress-dependent fracture transmissivity (“embedded fracture approach”). The approach was tested successfully for soft clays (bentonite) and for claystone. An even simpler approach based on a pressure-dependent permeability multiplier was introduced by Senger et al. (2008):

$$k = k_0 \left[1 + (k_{\text{factor}} - 1) \frac{(P - P_1)}{(P_2 - P_1)} \right] \quad (2-25)$$

where k_0 is the reference permeability, k_{factor} is a scaling factor, P_1 is the characteristic pressure for the onset of dilation, and P_2 is maximum pressure corresponding to the maximum permeability. Provided the porosity changes are considered negligible compared to the permeability changes, the relationship between capillary strength and permeability is typically represented by Leverett’s function as (Leverett 1941):

$$P_c = P_0 \sqrt{\frac{k_0}{k}} \quad (2-26)$$

or by a cubic-law function:

$$P_c = P_0 \sqrt[3]{\frac{k_0}{k}} \quad (2-27)$$

This simplified approach has been applied successfully for the interpretation of gas injection tests in the HG-D (Reactive Gas Transport in Opalinus Clay) experiment at Mont Terri (Marshall et al. 2013).

Romero & Gómez (2013) performed water and gas permeability tests in a triaxial cell on Opalinus Clay samples from Mont Terri and the Schlattingen borehole, as well as for samples of the clay-rich sequences (so-called «Brauner Dogger») from the Schlattingen borehole (see also Sections 3.2 and 3.3). A stress-dependent porosity (or void ratio) and permeability were identified in water injection tests under steep gradients (Fig. 2-7). Rapid gas-injection tests caused deformation of the clay due to the decrease in effective stresses, resulting in a change in “storativity” and, correspondingly, in porosity. This change in porosity and the associated change in permeability could be described as log-linear relationships of measured permeability and void ratios of core samples under different stress conditions. This behaviour represented a largely reversible elastic deformation, expressed by the bulk compressibility of the claystone as derived from isotropic compression tests. The analyses of air-injection tests demonstrated the importance of incorporating the coupled processes associated with the elastic behaviour of the claystone in terms of the stress-induced changes in porosity, permeability and capillary pressures on a local scale (Senger et al. 2014b). Further experimental evidence of hydro-mechanical coupling is given in Chapter 3.

Similar studies on the hydro-mechanical, one-dimensional behaviour of the Opalinus Clay from various sites and depths were carried out at LMS/EPFL (e.g., Ferrari et al. 2012, Ferrari et al. 2016 Favero et al. 2016). The stiffness parameters and the consolidation coefficient did show to be strongly dependent on the applied vertical stress. The comparison of the results obtained at the Laboratory of Soil Mechanics of the Swiss Federal Institute of Technology in Lausanne (EPFL/LMS) showed that the compressibility index C_c was in the range of 0.015 to 0.07, in which the lower values (thus stiffer material) were found for the deeper, shaly Opalinus Clay from the Schlattingen borehole (Ferrari et al. 2014) and the sandy Opalinus Clay from Mont Terri (Crisci et al. 2019). The swelling index C_s , the oedometric modulus E_{od} and the secondary compression coefficient C_α were found to increase with the applied vertical stress (up to 100 MPa), while the consolidation coefficient c_v was found to decrease. Stiffer responses were generally obtained for deeper or sandy Opalinus Clay. More details can be found in the aforementioned studies.

Crisci et al. (2019) as shown in Fig. 2-8, compared the hydraulic conductivity as a function of the void ratio of the Opalinus Clay (testing perpendicular to bedding) from the Lausen (Crisci et al. 2019), Mont Terri and Schlattingen boreholes (Favero 2017). The hydraulic conductivity of the tested specimens was shown to vary in the order of magnitudes of $10^{-12} - 10^{-14}$ m/s. The results showed a decrease in the hydraulic conductivity with the decrease of the void ratios, which, in turn, were related to mechanical compaction.

The anisotropic features of the shallow Opalinus Clay, in terms of oedometric compressibility and hydraulic conductivity, were investigated in Crisci et al. (2019). The results showed a significant difference of the elastic hydro-mechanical behaviour with regard to the loading directions, with a stiffer response and higher hydraulic conductivity in the direction parallel to bedding, while the elasto-plastic, hydro-mechanical behaviour was comparable. In other words, the anisotropic features were found to be reduced at high stress levels (post-yielding).

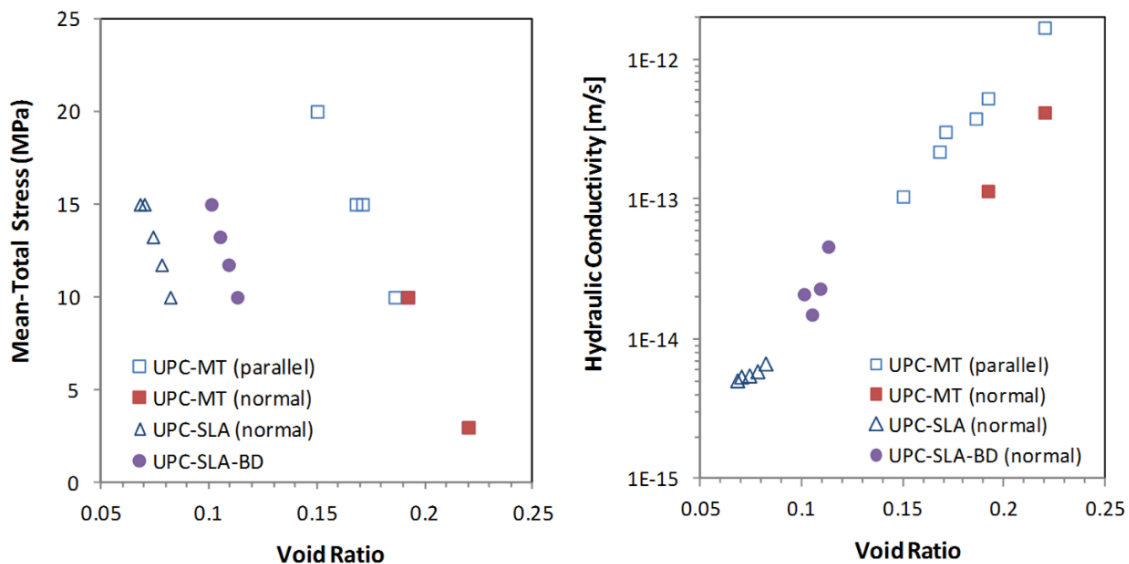


Fig. 2-7: Compressibility on isotropic loading of samples with flow parallel and normal to bedding (left). Results of the water-permeability tests on samples parallel and normal to bedding in terms of void ratio and hydraulic conductivity (right) (Romero et al. 2012)

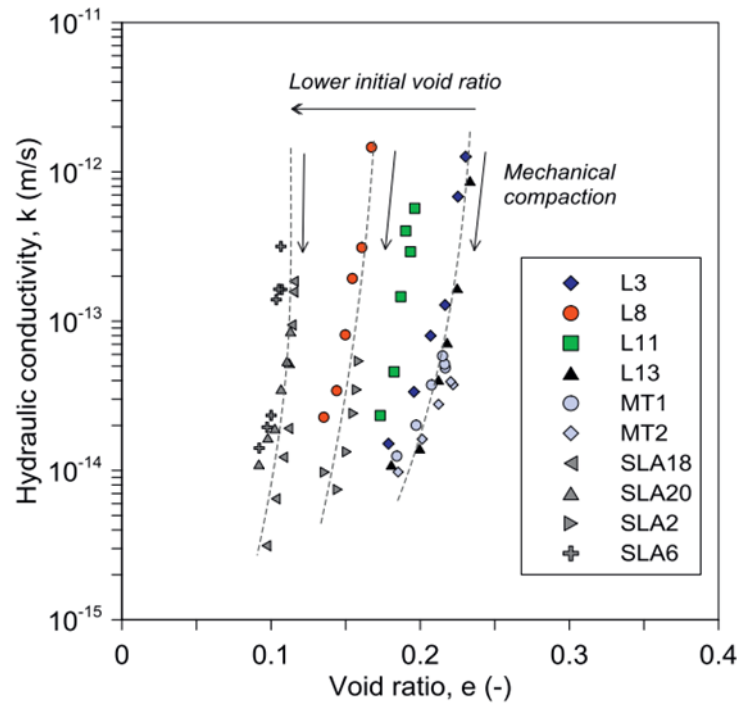


Fig. 2-8: Hydraulic conductivity, computed via consolidation theory of primary loading steps, versus void ratio

Comparison of the results of specimens from the Lausen, Mont Terri and Schlattingen boreholes (L-specimens) (from Crisci et al. 2019).

Empirical investigations and phenomenological descriptions of dilatancy-controlled gas flow through clay-rich seals were the subject of many geoscientific papers in the field of reservoir engineering (e.g., Clayton & Hay 1994, Ingram et al. 1997, Ingram & Urai 1999, Zweigel et al. 2005). Further evidence for pathway dilation phenomena has been found in other areas such as natural gas storage and CO₂ sequestration. Benson et al. (2002) reviewed the safety results of underground storage in the United States as part of a comprehensive study considering CO₂ storage in deep geological formations. The authors emphasised the importance of vertical pressure gradients as an indicator for the onset of dilatancy-controlled leakage through the cap rocks which cover natural gas storage formations. According to Ibrahim et al. (1970), the critical pressure gradient for dilatancy-controlled gas leakage is bracketed by the hydrostatic gradient ($\approx 9.8 \text{ kPa/m}$) and the lithostatic gradient ($\approx 22.6 \text{ kPa/m}$ assuming a bulk density of the overburden of about 2.3 g/cm^3), where the lithostatic pressure gradient represents a lower limit for the initiation of macroscopic fractures (cf. Section 2.2.4). It should be noted that the CSA Standard Z341 (CSA 2006) includes a recommendation that, in order to minimise the leakage rates, the maximum operating pressure of natural gas storage systems should not exceed 80% of the fracture pressure of the cap rock formation. In the absence of local fracture pressure data, a fracture gradient of 18.1 kPa/m is assumed, which leads to the maximum pressure gradient of 14.5 kPa/m (i.e., 80% of the fracture gradient). Further references with a collection of case studies on critical pressure gradients in the field of reservoir engineering are found in Evans (2008).

An important feature of the deformation behaviour of argillaceous materials is their self-sealing capacity (e.g., Nagra 2002). Permeability enhancement at elevated gas pressures tends not to be permanent; when the gas pressure is reduced, the material reconsolidates, and the hydraulic and mechanical properties of the porous medium approach the values which are characteristic for the undisturbed stress state.

Gas flow along macroscopic tensile fractures

In general, a macroscopic tensile fracture (hydraulic or gas fractures) develops when the gas pressure exceeds the sum of the minimum principal stress and the tensile strength of the rock (e.g., Valkó & Economides 1996). The brittle fracture is initiated quasi-instantaneously without precursory plastic deformation and propagates at about the velocity of a shear wave (e.g., Gross & Seelig 2007). Gas flow in such a macroscopic tensile fracture can be seen as a single-phase flow process. The propagation comes to a halt when the gas pressure in the fracture drops below that of the value of the minimum principal stress (shut-in pressure). Large hydraulic fractures are characterised by a fracture transmissivity which increases the bulk permeability of the rock by many orders of magnitude. In a rock with low tensile strength, a macroscopic fracture develops only when the gas pressure build-up is rapid, i.e., when the combined effect of porewater displacement and formation of small-scale fractures (i.e., dilatancy) no longer counterbalances the gas production rate.

The conceptual, theoretical and experimental framework for fracture propagation is well documented in standard hydrocarbon exploration literature (e.g., Valkó & Economides 1996).

2.3 Modelling of gas transport processes in heterogeneous media

2.3.1 Basic modelling approaches

For any of the aforementioned mechanisms, gas transport is controlled by the microscopic structure of the porous medium. Subscale variability of the void space may have a distinct impact on transport processes at scales exceeding the characteristic length of the heterogeneities by orders of magnitudes. In the assessment of gas release from a deep geological repository, scales are an issue not only for gas pathways through the intact rock matrix, but also for gas release in fracture networks (fractured host rocks such as the Effingen Member; gas transport along the excavation-damaged zone around the backfilled underground structures).

The modelling concepts reported in the scientific literature for the simulation of two-phase flow processes in porous media are based on two different fundamental approaches:

- *Discrete pore network models (channel networks or fracture networks)* represent the porous medium as a network of connected channels. At a given location, a channel is occupied either by the wetting or by the non-wetting fluid. Flow in the channels occurs by piston-like displacement as a result of the pressure difference between the phases. Fluid displacement is simulated by simplified invasion percolation (IP) algorithms. Frequently, stochastic approaches are adopted to describe the geostatistical properties of the porous medium at the pore scale. Such stochastic discrete network models have been applied successfully for the simulation of two-phase flow processes in the regime of capillary fingering (Glass & Yarrington 2003, Lenormand & Zarcone 1989). The main challenge is the realistic geostatistical description of the pore network in a stochastic framework, which requires comprehensive microstructural databases for the model identification and conditioning process.

- *Equivalent porous medium models* are based on the classical mixing theory of continuum mechanics of fluids (e.g., Coussy 2004). In this concept, the three phases (solid, wetting fluid, non-wetting fluid) are assumed to superimpose each other at a given location of the porous medium. Basic physical principles, such as mass and momentum balance and the laws of thermodynamics, apply for each phase and for all types of energy transformation in the system. The phases are described in terms of continuous density functions, implying that a representative elementary volume exists, which is relevant for all the physical phenomena involved in the intended application at the macroscopic scale. On this scale, phase couplings are expressed in terms of capillary pressure and relative permeability-saturation relationships. Numerous scientific papers have been published in recent years, aimed at assessing the range of validity of the continuum models of two-phase flow (Artus & Noetinger 2004, Jacobs & Gelhar 2005, Stauffer et al. 2009, Neuweiler et al. 2011).

2.3.2 Gas transport in channel networks and fracture networks

Claystones exhibit low permeability, low porosity and a pore-size distribution consisting mainly of micropores (< 2 nm) and mesopores (2 – 50 nm). The low permeability is associated with low capillary numbers, suggesting that gas transport occurs in the regime of capillary fingering. The displacement of porewater by a gas phase is mainly restricted to the sparse network of macropores (> 20 nm), because the micro- and mesopores are hardly invaded by the gas phase due to their high capillary entry pressure. The poor connectedness of the network of macropores raises the issues of the appropriate averaging volume (“representative elementary volume”) and, as a consequence, of the transferability of the equation of motion from a local (pore) scale to a global scale formulation, which can be expressed in terms of macroscopic “effective” two-phase flow properties of the equivalent porous medium.

Valuable insight addressing the issue of spatial continuity of the pore structure can be gained by high-resolution 3D imaging techniques such as transmission electron microscopy (TEM), focussed ion beam nanotomography (FIB-nT) and microcomputed tomography (micro-CT) (Keller et al. 2011, Keller et al. 2013a).

Keller et al. (2013b) performed geostatistical analyses on Opalinus Clay samples (Fig. 2-9), which had been subjected to comprehensive microstructural characterisations (TEM, FIB-nt, scanning electron microscopy (SEM)) at scales ranging between 5 nm and 500 µm. Local porosity distributions and directional percolation probabilities were inferred, drawing on the conceptual framework of local porosity theory (Biswal et al. 1998). Keller et al. (2013b) concluded that the porosity of the Opalinus Clay samples homogenises at sample sizes > 10 µm³, which defines the order of magnitude of the REV (representative elementary volume). Percolation probability of the Opalinus Clay samples displayed a marked variability and a distinct anisotropy, indicating enhanced connectivity parallel to bedding. Connectivity perpendicular to bedding was generally poor. However, the analysed database was still too small for a reliable geostatistical interpretation of the directional percolation probability.

In fractured rock such as the Helvetic Marls and the Effingen Member, gas transport is essentially restricted to the porosity associated with the fracture systems, whereas the pore space of the intact rock matrix is not accessible for gas. The complexity of the fracture systems in terms of geometry and hydraulic characteristics prevents deterministic approaches and favours stochastic representations of the fracture systems. In the context of the Wellenberg programme (Nagra 1997), a stochastic fracture network model of the Helvetic Marls at the Wellenberg site was elaborated. The model was conditioned with logging data and packer test results from the site investigation programme and served as a tool for converting fracture transmissivities at the scale

of the borehole investigations into effective hydraulic conductivity values on the block scale with typical block sizes $\geq 50 \mu\text{m}^3$. Eventually, the block conductivities fed into a stochastic groundwater flow model for simulating porewater flow at the repository scale.

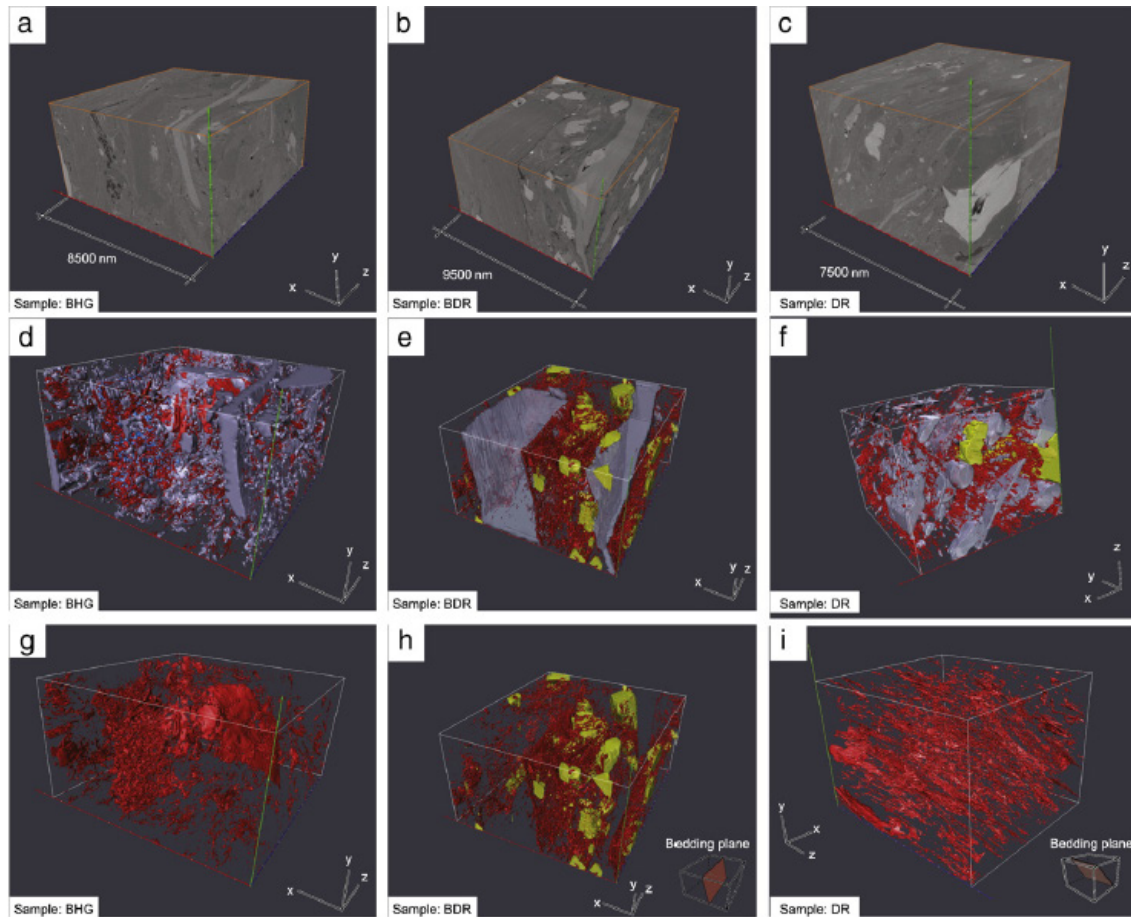


Fig. 2-9: Stages of FIB-nt data processing of three rock samples recovered from the Mont Terri URL (BHG – left, BDR – middle and DR – right) by Keller et al. (2011)

Pictures (a), (b) and (c) show the 3D reconstruction of the analysed volume. Pictures (d), (e) and (f) present the 3D visualisation of the segmented microstructure. The volume is separated into four categories: (i) pores (red), (ii) calcite (yellow), (iii) large mineral grains (grey) and (iv) matrix (transparent). Pictures (g), (h) and (i) display the 3D microstructure of the pore space. Note the strongly preferred orientation of elongated pore objects in the DR sample. The cubes in (h) and (i) indicate the orientation of the bedding plane.

Wettstein et al. (2011) made use of the aforementioned stochastic fracture network model (Fig. 2-10) to derive a representative water retention behaviour of the Helvetic Marls as input for repository-scale modelling of gas release at the Wellenberg site. They adopted an invasion percolation (IP) algorithm to invade the fracture network with a non-wetting fluid. Fluid invasion was controlled by the gas entry pressure of the individual fractures, derived from fracture transmissivity according to equations (2-11) and (2-12b):

$$P_{ae} = 4 \cdot \sigma_{gw} \cdot (12\mu T)^{-1/3} \cdot \cos \alpha \quad (2-27)$$

Multiple stochastic realisations of the Wellenberg fracture network model were subjected to the IP analysis by the stepwise increase of the fluid pressure and determination of the corresponding fluid volume. Thus, pressure-saturation curves could be derived for each stochastic realisation of the fracture network. Finally, the ensemble average of the derived pressure-saturation curves was calculated, representing the effective water-retention curve of the Helvetic Marls at the block scale (Fig. 2-10).

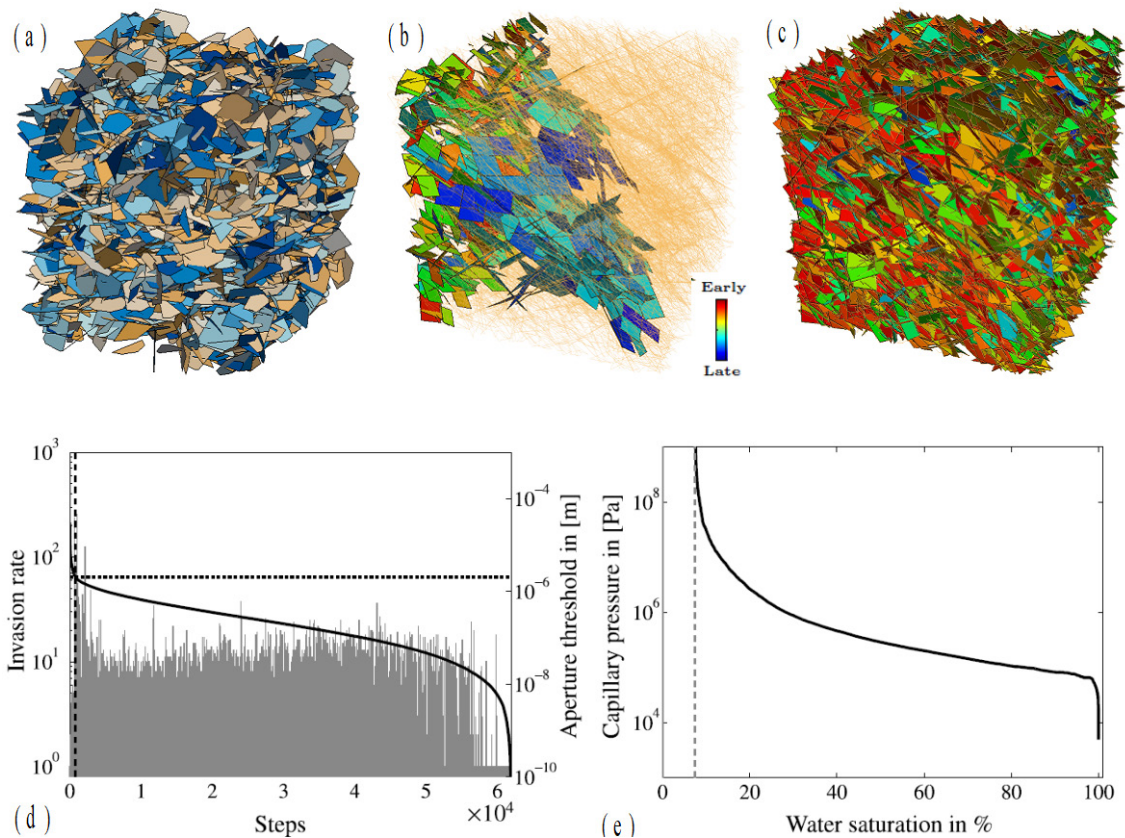


Fig. 2-10: Characterisation of the water-retention behaviour of fractured rock after Wettstein et al. (2011)

(a) Stochastic fracture network representation of the Helvetic Marls at the Wellenberg site after Nagra (1997). Colour coding of fractures reflects fracture transmissivities in relative units. (b) Invaded fractures at breakthrough marked from early to late invasion. (c) Invaded fractures after full invasion. (d) Invasion rate (e) Derived capillary pressure-saturation relationship.

The stochastic realisations of the discrete fracture network (DFN, Fig. 2-10a) were transformed into equivalent representations of a continuous porous medium (CPM), basically following the approach of the so-called Wellenberg K-model (Nagra 1997). Equivalent properties of CPM elements were calculated from each DFN realisation using the upscaling method of Jackson et al. (2000), which is implemented in the CONNECTFLOW code Lanyon & Senger (2011). This method calculates the equivalent permeability tensor for subregions of the DFN by fitting the flow rates (as calculated in the DFN model) across the subregion for different hydraulic gradients. In the current application, an equivalent tensor has been calculated for each cell in the CPM model. The CONNECTFLOW CPM representation was converted into a TOUGH2 model as described in Lanyon & Senger (2011).

2.3.3 Gas transport in porous media with stochastic property distributions

In the regime of capillary fingering, the spatial variability of porosity and permeability has a strong impact on the invasion of the non-wetting fluid (see Section 2.2.2). Gas release from the backfilled repository structures through the host rock with a typical capillary numbers log of $C_a < -10$ and a mobility ratio log of $M \approx -2$ takes place in the regime of capillary fingering. Therefore, the impact of spatial variability of the rock properties has to be addressed when gas transport processes are simulated in the host rock around the repository.

Papafotiou et al. (2011) conducted generic modelling studies, aimed at quantifying the impact of the spatial variability of rock properties on gas release through the host rock on a deca- to hectometre scale. Simulations were conducted for the stochastic property distributions and for the corresponding homogeneous property models. A good agreement of the calculated distributions of pressure and saturation was achieved for those cases with moderate property variability (i.e., Opalinus Clay), whereas significant differences were seen for the Effingen Member. In all cases, the stochastic simulations provided a more realistic picture of the gas release processes around the disposal systems in that they account for phenomena such as gas entrapment and gas flow localisation (capillary fingering).

3 Gas-related properties of clayey rock formations

3.1 Relevant rock properties and constitutive relationships

A comprehensive set of geotechnical rock properties and constitutive relationships is required for the numerical simulation of gas transport processes in the host rock formations. Chapter 3 provides an overview of the rock properties of concern, the underlying data sources and the derived reference parameters required for numerical simulations of gas release through the candidate host rocks.

The following parameters are required for modelling gas transport processes in the host rock formations:

- Total porosity and the associated microstructural features of the pore structure (e.g., pore-size distribution), governing both the gas storage and the gas transport capacity.
- Intrinsic permeability, characterising the transport capacity of the host rock independent of the fluid.
- Capillary pressure, characterising the coupling between gas and water pressure as a function of saturation.
- Relative permeability, characterising the mobility of the different phases as a function of saturation.
- Critical pressure for the onset of pathway dilation, separating the regimes of reversible and irreversible deformation.

3.2 Opalinus Clay

3.2.1 Basic geological characteristics of the Opalinus Clay formation

The Opalinus Clay is part of a thick Mesozoic – Tertiary sedimentary sequence in the Molasse Basin of Northern Switzerland. It was deposited about 170 Ma ago in a shallow marine environment. Geological investigations on the regional scale confirmed the remarkable homogeneity of the formation. In the potential siting regions of Northern Switzerland, the Mesozoic sediments reveal a uniform thickness over a distance of several tens of kilometres, dipping gently to the southeast, and are hardly affected by faulting (see Nagra 2024b for further information).

The Opalinus Clay is a moderately overconsolidated claystone that has been formed by a complex burial and compaction history with two distinct periods of subsidence during the Cretaceous and late Tertiary, respectively. In the Molasse Basin, the greatest burial depth of the Opalinus Clay was about 1,000 m below the present depth. From about 10 Ma ago, alpine uplift and erosion brought the Opalinus Clay progressively up to its present burial depth.

On a regional scale, the mineralogical composition of the Opalinus Clay exhibits moderate lateral variability and a slight increase in clay content with depth. Quantitative laboratory analyses of core samples from the deep boreholes and Mont Terri provide a total mass fraction of clay minerals of 40 – 80%, a quartz content of 15 – 35% and 5 – 25% carbonates (Fig. 3-1). The fraction of swelling clay minerals, with 10 – 15% illite/smectite mixed layers, is of particular interest for the gas-related studies. Further minerals are siderite, pyrite and feldspar. The mass fraction of organic carbon is < 1%.

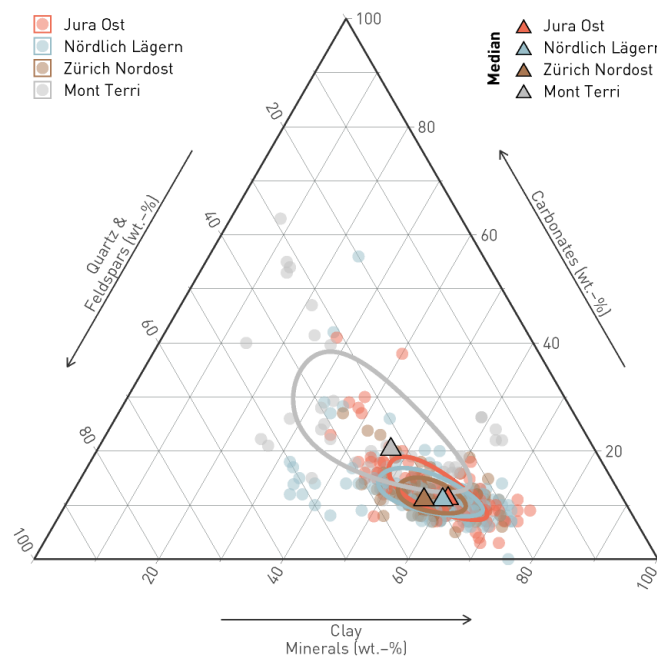


Fig. 3-1: Mineralogical composition of the Opalinus Clay

Data are shown for all boreholes from the most recent deep borehole campaign and from Mont Terri (Nagra 2024b).

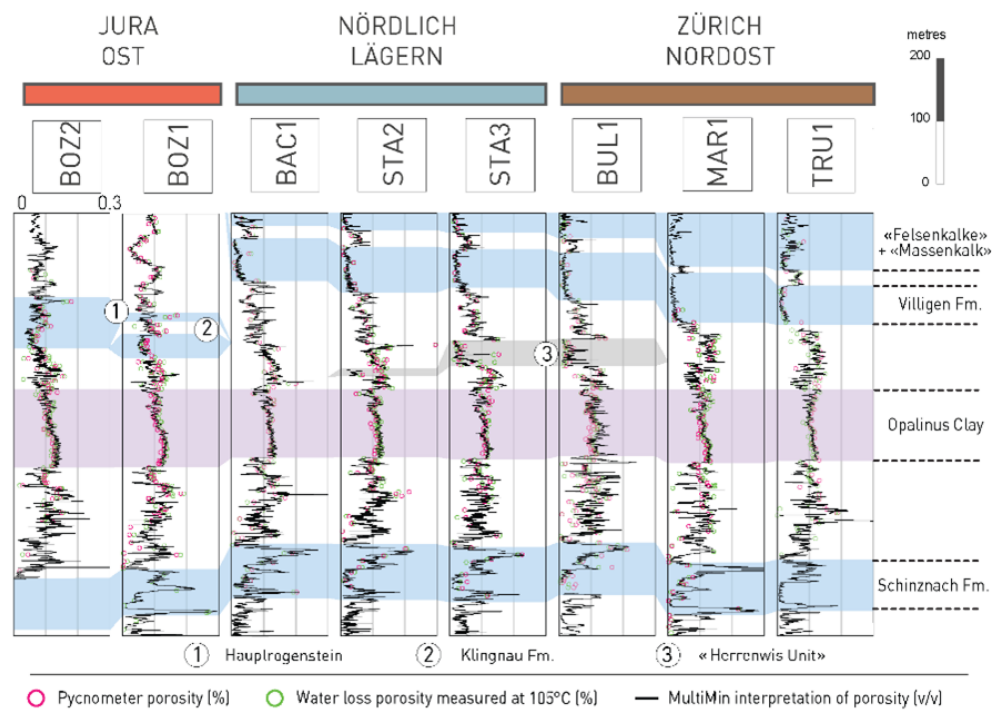


Fig. 3-2: Porosity profiles from selected boreholes

(From Nagra 2024b).

Porosity and pore-size distribution are relevant determining factors for a number of rock properties, such as permeability, diffusion and various geomechanical parameters and moduli. The Opalinus Clay is characterised by a relatively large porosity but, at the same time, extremely small pore apertures. The typical range for porosity in the Opalinus Clay in the potential siting regions is 0.10 – 0.13. In the continuous log-derived porosity profiles, Opalinus Clay is visible as a zone of little variation (Fig. 3-2). At Mont Terri, porosity is somewhat higher (0.12 – 0.14), which can be explained by the external position relative to the Alpine front and therefore a less deep Miocene burial and compaction. There is a moderate correlation between the current depth of the Opalinus Clay and its porosity (Fig. 3-3).

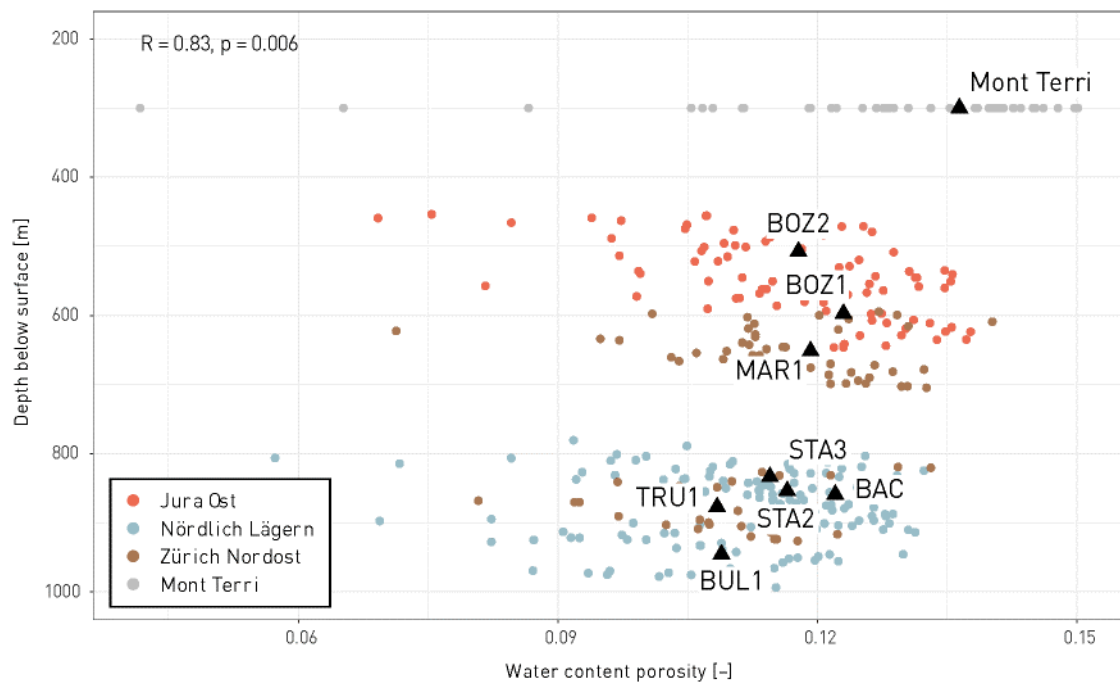


Fig. 3-3: Water-loss porosity of the Opalinus Clay in different boreholes as a function of current depth
(From Nagra 2024b).

Further geotechnical characteristics of the Opalinus Clay have been determined as part of comprehensive laboratory programmes, revealing moderate stiffness (Young's modulus in the range of 5 – 15 GPa), moderate strength (unconfined compressive strength (UCS) values of the intact rock matrix between 10 and 35 MPa) and distinct swelling pressures (0.5 – 2 MPa).

A comprehensive and robust database regarding the hydraulic properties has been compiled (Nagra 2024b), comprising data from TBO investigations in the three siting regions as well as from earlier investigation programmes, from the Mont Terri URL and from third-party investigations. Hydraulic properties are known to depend on overburden. In the Opalinus Clay, high values up to ca. 10^{-4} m/s are observed only in the uppermost decametres (Fig. 3-4) due to rock weathering and decompaction. With increasing depth, the values decrease by several orders of magnitude, e.g., in the Mont Terri URL typical values are in the range of 1×10^{-12} to 1×10^{-13} m/s. The best estimates of the average hydraulic conductivities from hydraulic packer tests carried out in the deep boreholes drilled in the JO, NL and ZNO siting regions plot in the narrow range, namely from 1×10^{-13} to 1×10^{-14} m/s. At this overburden, no depth dependence is visible.

During the TBO campaign, hydraulic testing of fractures (faults, joints) was a primary test target in all boreholes. The histogram of the (interval) transmissivities shows the generally low values of approximately $1 \times 10^{-12} \text{ m}^2/\text{s} \pm$ one order of magnitude (Fig. 3-5). The maximum value of $10^{-11} \text{ m}^2/\text{s}$ is from a long test interval at the base of the Opalinus Clay in the Schafisheim borehole. This interval includes a major fault zone related to the folding and thrusting of the Jura Mountains – such structures are absent in the siting regions.

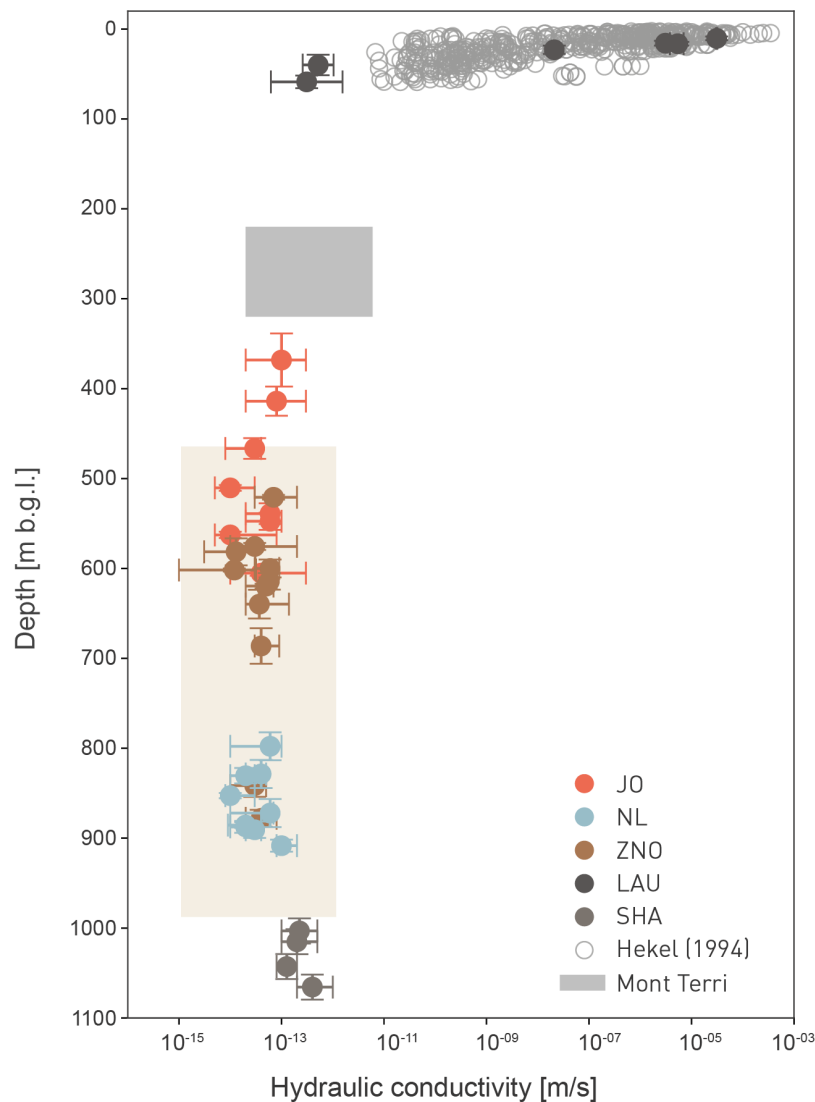


Fig. 3-4: Hydraulic conductivities of the Opalinus Clay as a function of depth (From Nagra 2024b).

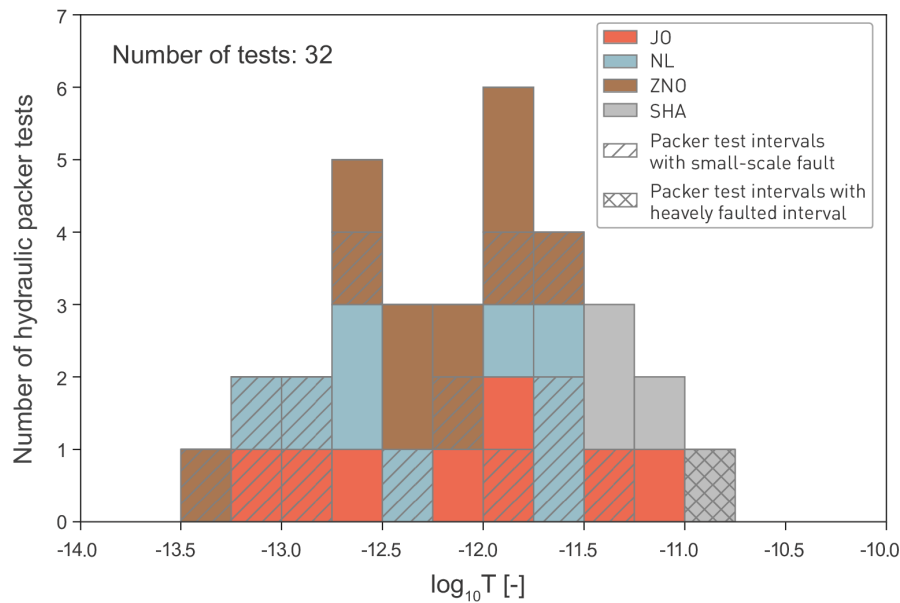


Fig. 3-5: Distribution of transmissivity from in-situ tests in the Opalinus Clay (From Nagra 2024b).

Over the course of the Mont Terri research programme, a comprehensive hydrogeological investigation programme has been conducted. Some of the key achievements on porewater flow in the Opalinus Clay were summarised in Bossart & Thury (2008):

- The highest packer test transmissivities recorded for the Opalinus Clay at Mont Terri, which cannot be explained by EDZ phenomena, are $< 1 \times 10^{-10} \text{ m}^2/\text{s}$. Hydraulic packer testing in boreholes and permeameter testing with drill-core specimens exhibit consistently low values for hydraulic conductivity, typically in the range between 5×10^{-12} and $1 \times 10^{-14} \text{ m/s}$ (see also Nagra 2014b). No significant variations in hydraulic conductivity are seen among the different facies. A reference value of $5 \times 10^{-13} \text{ m/s}$ has been reported for the Opalinus Clay at Mont Terri.
- No marked enhancement of hydraulic conductivity has been measured in the vicinity of tectonic features, indicating that fractures in the Opalinus Clay are tight. Extensive packer testing in the main fault did not reveal any correlation between hydraulic conductivity and fracture frequency along the boreholes.

3.2.2 Gas-related characteristics of the Opalinus Clay

Gas transport in low-permeability formations is largely controlled by the microstructure of the rock. A balanced assessment of gas transport processes in the Opalinus Clay therefore requires careful consideration of both structure and texture. Fig. 3-6 illustrates the mineralogical and structural features of the Opalinus Clay in the ZNO siting region at various scales. Petrophysical logs in the Benken borehole indicate moderate variability and a slight increase of clay content with depth, suggesting a division of the Opalinus Clay into five lithostratigraphic subunits (facies). Core inspection reveals a distinct anisotropy, made up of siderite concretions and silt and sandstone lenses, which are embedded in the clay-rich strata. The anisotropy due to bedding is largely a result of microscopic heterogeneity as seen in the thin sections, where diagenetic cementation of the pore space has been observed in the silty and sandy layers. SEM images reveal that the size of the mineralogical components ($10^{-7} - 10^{-3} \text{ m}$) determines the microstructure of the

rock. Quartz minerals can exhibit grain sizes in the range 0.01 – 1 mm, whereas the clay minerals form flake-like packages with typical sizes in the order of 100 nm – 10 µm. The pore space of the rock is formed by a network of micro-, meso- and macropores, which is too small (in the order 1 – 100 nm) to be shown by conventional SEM methods. This network of pores actually dominates the flow and transport properties of the rock (see also Appendix A in Senger et al. 2013).

Tab. 3-1: Volume fractions of the different pore classes, determined by adsorption and desorption isotherms (H₂O, N₂) after Nagra (2002)

Complementary experimental evidence suggests that at least 20% of the total porewater can be attributed to the interlayer water.

Equivalent radius [nm]	Micropores < 1	Mesopores 1 – 25	Macropores > 25
Assumption: fraction of micropores is 20% (interlayers)			
N ₂ isotherm	20	46 – 56	24 – 35
H ₂ O isotherm	20	54 – 63	17 – 26

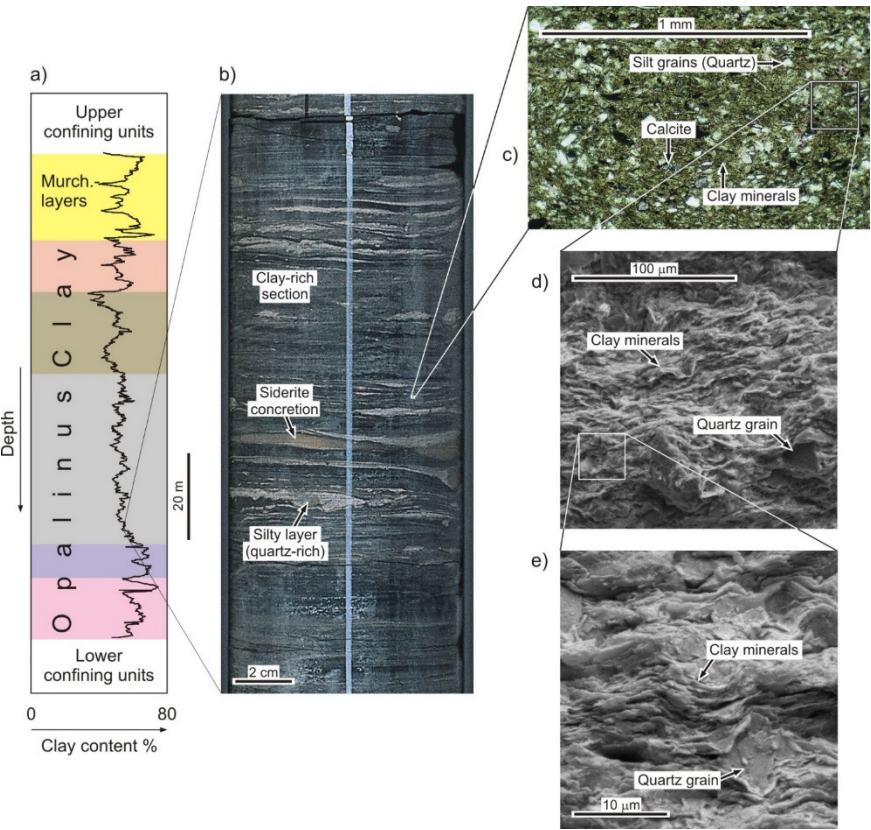


Fig. 3-6: Illustration of the mineralogy and structure of the Opalinus Clay at different scales, based on data from the Benken borehole in the ZNO siting region

(a) Vertical profile of clay content determined by petrophysical logging; (b) core sample; (c) thin sections; and (d, e) SEM images (after Nagra 2002).

Consistency limits

The consistency limits were investigated at the Universitat Politècnica de Catalunya (UPC) in Barcelona, Spain, and the EPFL/LMS for Opalinus Clay samples from shallow and deep sites. In the context of the EURAD GAS project, UPC measured a liquid limit (w) of 28.1% and a plasticity limit (w) of 21.5% for the OPA-881 sample, resulting in a plasticity index of 6.6%, while values of 27.6% and 21.8%, respectively, were obtained for the OPA-929 sample, resulting in a plasticity index of 5.8%. Fig. 3-7 shows the plasticity chart, which also includes consistent results reported by different authors at similar depths (Ferrari et al. 2014, Gonzalez-Blanco 2017). According to the plasticity chart, deep Opalinus Clay can be classified as an inorganic clay with low to very low plasticity and no or low dilatancy.

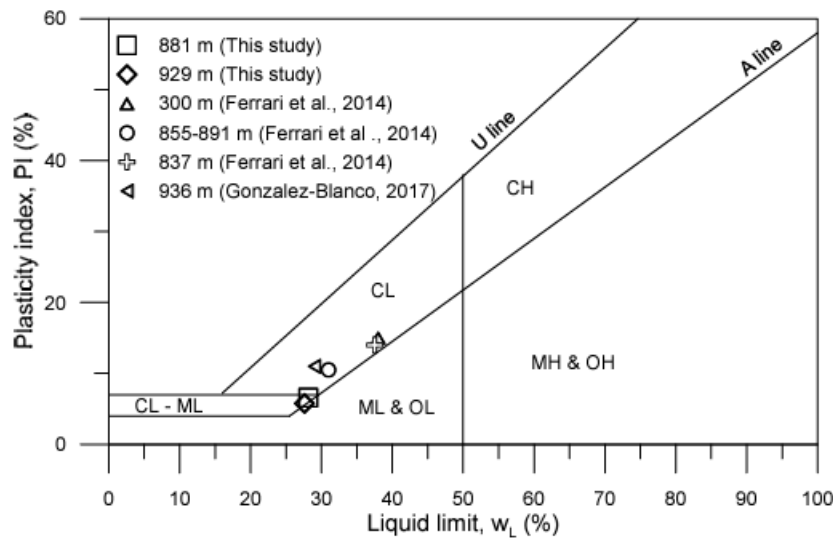


Fig. 3-7: Plasticity chart – Opalinus Clay from different sites

Pore-size distribution

Complementary methods were used to characterise the pore space of the Opalinus Clay, such as the measurement of the adsorption/desorption isotherms and mercury porosimetry (Nagra 2002). To obtain nitrogen and water isotherms, the powder samples were dried at temperatures of at least 120 °C and degassed under a vacuum. Nitrogen isotherms were measured at 77 K and water isotherms at 303 K by gravimetry in quasi-equilibrium mode, where water vapour was introduced at a constant, low flow rate. The pore-size distributions were obtained by incremental saturation of the sample. Fig. 3-8 depicts the volume fractions of the different pore classes (definition according to IUPAC 1997), indicating that the majority of pores can be classified as mesopores (1 – 25 nm). The inferred macropore fraction in the order of 20 – 30% represents the pore space relevant for gas transport as these pores are accessible to gases at moderate gas pressures (cf. Young's Equation 2-12).

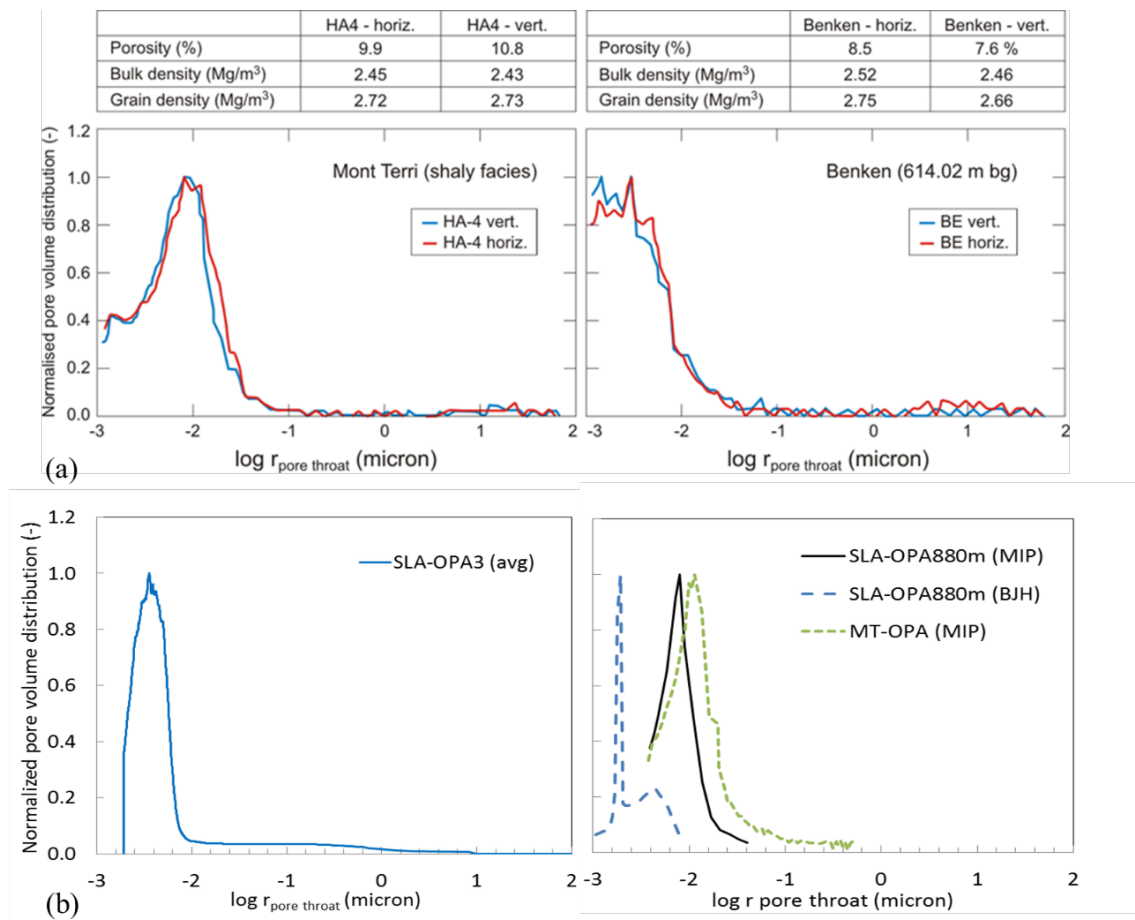


Fig. 3-8: Equivalent pore-size distributions of drill-core samples

(a) From Benken (sampling depth 614.82 m below ground) and Mont Terri (shaly facies), determined by mercury intrusion methods at Chevron's laboratories in Houston, Texas, USA (courtesy of Philip Mariotti); (b) from Schlattingen (sampling depth 880 m below ground), determined by mercury intrusion methods at EPFL (left) and UPC (right), complemented with the BJH method.

For mercury porosimetry, Hg was injected at increasing pressures into crushed, dried and degassed samples. In the context of the demonstration of disposal feasibility, i.e., Project *Entsorgungsnachweis* (Nagra 2002), the maximum injection pressure was 200 MPa, and thus only pores with a radius larger than 3.7 nm could be detected. As part of Nagra's collaboration with the oil and gas industry, new mercury-intrusion experiments were conducted in 2004 at the geotechnical laboratories of Chevron in Houston by Philip Mariotti using injection pressures up to 420 MPa. Two core samples from Benken and Mont Terri were tested, and the equivalent pore-size distributions are shown in Fig. 3-8a. The general distributions are consistent with the results of the adsorption/desorption measurements, indicating that the majority of pores in the Opalinus Clay can be classified as mesopores. The more detailed comparison of the cores from Benken and Mont Terri reveals that the pore-size distributions of the core samples from Benken shift towards the lower pore radii. This is a clear indication of the higher degree compaction of the samples from Benken, corresponding to the higher burial depth. More recent analyses were performed on core samples from a depth of 880 m in the Schlattingen borehole by EPFL and UPC, shown in Fig. 3-8b. UPC complemented the analyses using the mercury intrusion porosimetry (MIP) method

with the BJH (Barrett, Joyner and Halenda) method, using the desorption information from the nitrogen adsorption tests. This provides a wider range of pore size, whereby the spike of around 0.004 micron is an anomaly due to the evaporation of metastable pore fluid (Romero et al. 2012).

New MIP analyses were carried out in the context of the TBO programme. Tests on the Opalinus Clay were performed by EPFL (Fig. 3-9) and UPC/CIMNE (Fig. 3-10) in the context of the EURAD-GAS project on core materials from the deep boreholes Trüllikon, Bülach and Bözberg. Those materials are located in-situ at different depths; they differ significantly from the shallow location at Mont Terri, indicating different geotechnical characteristics and hydro-mechanical behaviour in terms of geological burial history.

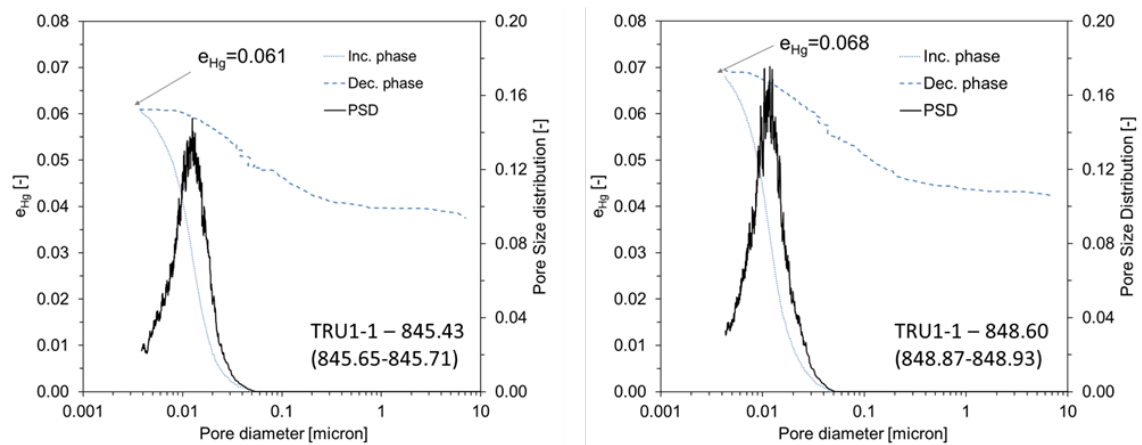


Fig. 3-9: MIP results for core material from the Trüllikon borehole (TRU1-1) by EPFL

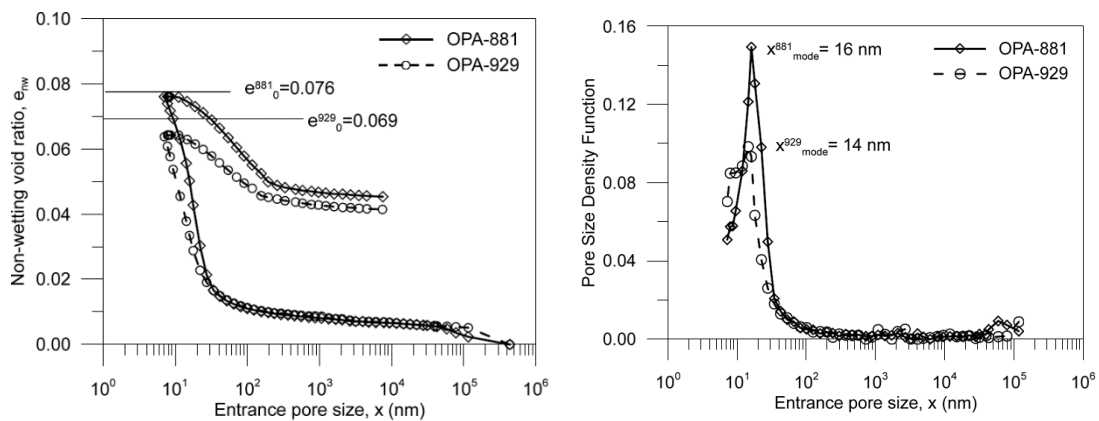


Fig. 3-10: MIP results for cre material from the Bülach borehole (BUL 1-1) by UPC

(a) Cumulated non-wetting void ratio gained with the MIP technique for different entrance pore sizes; (b) pore-size density (PSD) functions derived for samples BUL 1-1-OPA 881 and OPA 929.

Water-retention behaviour

Water-retention functions describe the capacity of a porous medium to retain water at a given suction head. Thus, the water-retention function is, in principle, identical to the water-adsorption isotherm. The main differences are the experimental procedure and the preparation of the samples. Water-retention curves of the Opalinus Clay were determined at the geotechnical laboratories of UPC, by stepwise desaturation and resaturation of core samples under controlled humidity (Nagra 2002, Muñoz et al. 2003). A comprehensive experimental programme was accomplished by the laboratories of Germany's central expert organisation in the field of nuclear safety and radioactive waste management (GRS), aimed at comparing the capillary pressure-saturation relationships of different clay formations. More recently, the Laboratory for Soil Mechanics at EPFL and the Department of Geotechnical Engineering and Geosciences at UPC determined water-retention curves as well as the hydraulic and geomechanical properties of core samples from Mont Terri and from a deep borehole (Ferrari & Laloui 2012, Ferrari et al. 2012, Romero & Gómez 2013). Fig. 3-11 depicts a compilation of water-retention curves of Opalinus Clay samples from Mont Terri, determined by GRS (Zhang & Rothfuchs 2007), by UPC (Muñoz et al. 2003, Romero & Gómez 2013), and by EPFL (Ferrari et al. 2012). Water-retention curves of deep Opalinus Clay core samples (from a depth of 880 m from the Schlattigen borehole) are shown in Fig. 3-12 using the FDT (fluid displacement technique with Kerdane) method for the volumetric determination of the specimen and for the determination of the suction as a function of water content and void ratio. The water-retention curves in Fig. 3-13 were based on the progressive method (Ferrari et al. 2012), where the wetting and drying paths of the retention curve are obtained on one single specimen from a core. This method better reproduces the hysteretic behaviour compared to the FDT method, where the data points are from different specimens, resulting in greater scatter (Fig. 3-13).

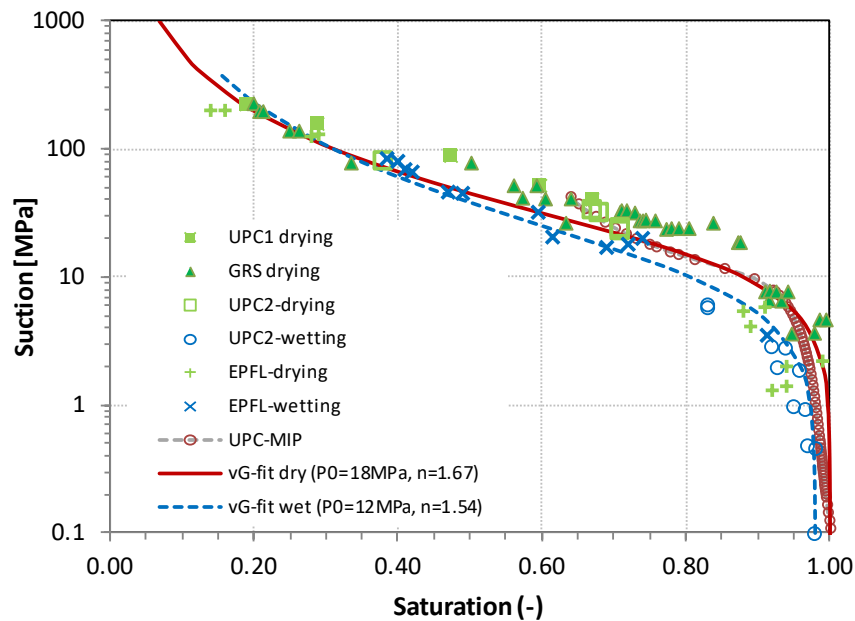


Fig. 3-11: Capillary pressure measurements (water-retention curves) by stepwise desaturation and resaturation in a desiccator

The experiments were conducted by GRS (Zhang & Rothfuchs 2007), UPC (Muñoz et al. 2003, Romero & Gómez 2013) and EPFL (Ferrari & Laloui 2012).

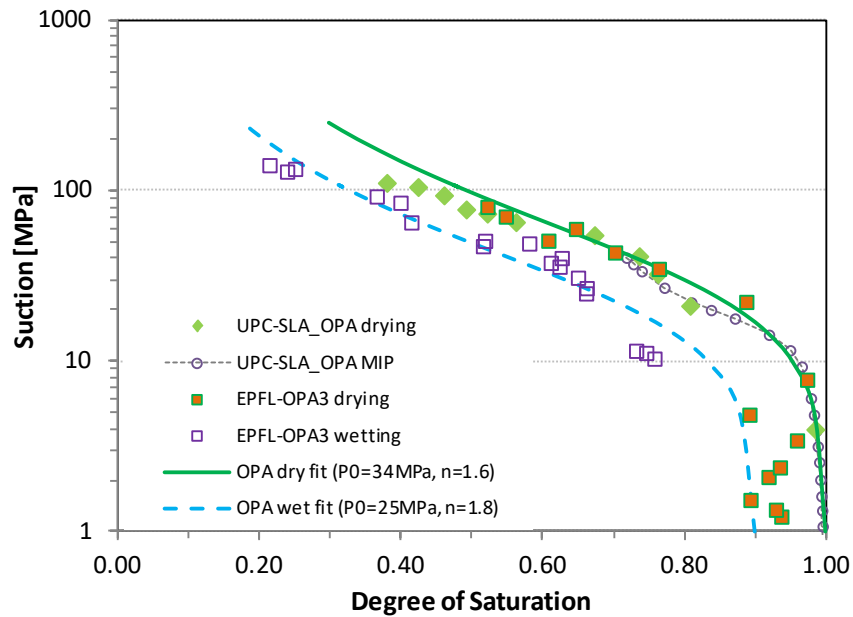


Fig. 3-12: Capillary pressure measurements (water-retention curves)

This was achieved by means of stepwise desaturation and resaturation using a WP4c dew-point psychrometer and volumetric measurements using the Kerdane method on deep core samples of the Opalinus Clay from the Schlattingen borehole (Ferrari et al. 2012, Romero & Gómez 2013).

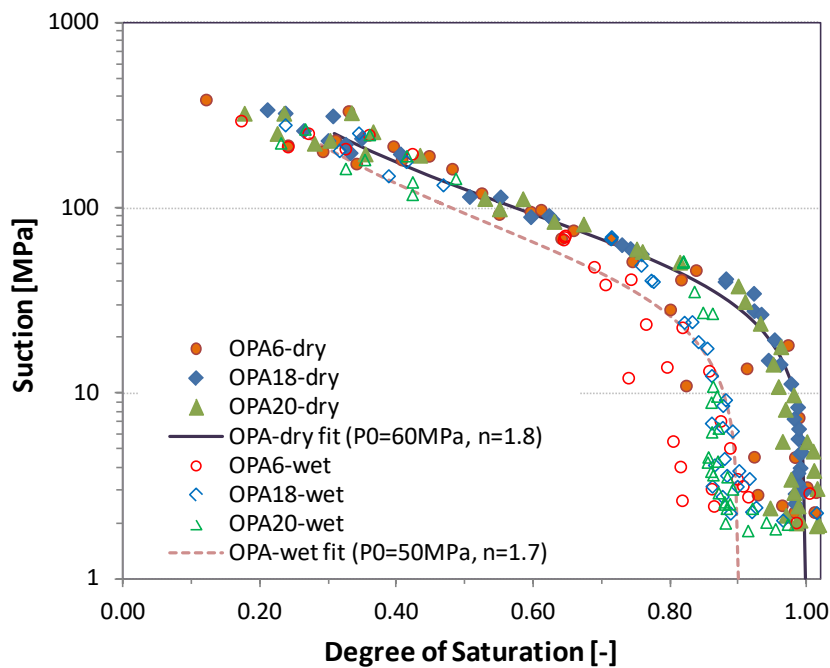


Fig. 3-13: Capillary pressure measurements (water-retention curves)

Results were achieved by stepwise desaturation and resaturation using a WP4c dew-point psychrometer and volumetric measurements using the progressive method on a deep core sample of the Opalinus Clay from the Schlattingen borehole (Ferrari et al. 2012).

Gas and liquid mobility (relative permeability-saturation relationship)

The mobility of the gas in the intact Opalinus Clay (expressed in terms of a relative permeability relationship) can be determined by water and gas permeameter experiments in the laboratory and by in-situ gas-injection tests in boreholes. A first experimental database for the derivation of relative permeabilities of the intact Opalinus Clay was elaborated in the context of the demonstration of disposal feasibility, Project *Entsorgungsnachweis*. The key references of previous experiments are given in Nagra (2002) and in Marschall et al. (2005). Further experiments and data analyses were compiled as part of the Mont Terri Project (Poller et al. 2008, Croisé et al. 2006) and in the context of the EU-funded integrated project NF-PRO (<http://www.nf-pro.org/>).

In the context of Stage 2 of the SGT, a complementary test programme was started, drawing on Opalinus Clay core samples from Mont Terri ("shallow samples") and from the Schlattingen borehole ("deep samples"). The tests were conducted in a triaxial cell with flow direction parallel (shallow samples only) and perpendicular to bedding at isotropic stress levels of 15 and 19 MPa, respectively (Romero & Gómez 2013). The corresponding gas-injection pressures (14 and 18 MPa, respectively) remained below the confining stress. Fig. 3-14 presents the results of the two gas injection tests on the core sample OED/Opalinus Clay (879.79 – 880.01 m) from the Schlattingen (SLA-1) borehole in terms of gas pressures at the injection and outflow sides together with outflow volume and axial displacements. A further gas-injection test was carried out on a core sample from the same borehole, recovered from a depth of 936 m b.g.l. Fig. 3-15 compares the transients of pressure, outflow rate and strain of the two tests, indicating a very similar behaviour.

The water/air permeability experiments on the Opalinus Clay sample show clear evidence for the dependency of water permeability on void ratio and thus on constitutive stress (estimated as the isotropic stress minus the air pressure at the injection point; see also Section 3.2.5). Furthermore, a marked dependency of gas dissipation was observed in the direction of gas flow with respect to bedding orientation. Significantly higher gas flow rates were observed for the flow direction parallel to bedding. Another important observation is the marked dependency of volumetric strain on the constitutive stress changes during air-injection and dissipation tests. The samples displayed expansion at the early rapid air-injection stage in response to a decrease in constitutive stress, and dominant compression on air-pressure dissipation. During the early period after shut-in, the axial strain continued to expand despite the slight increase in constitutive stress due to air dissipation. This phenomenon occurred under an increasing amount of air stored in the sample before the development of an air-driven opening of discontinuities. Higher bulk moduli were consistently obtained in the air-dissipation phases compared to bulk moduli from loading and unloading stages.

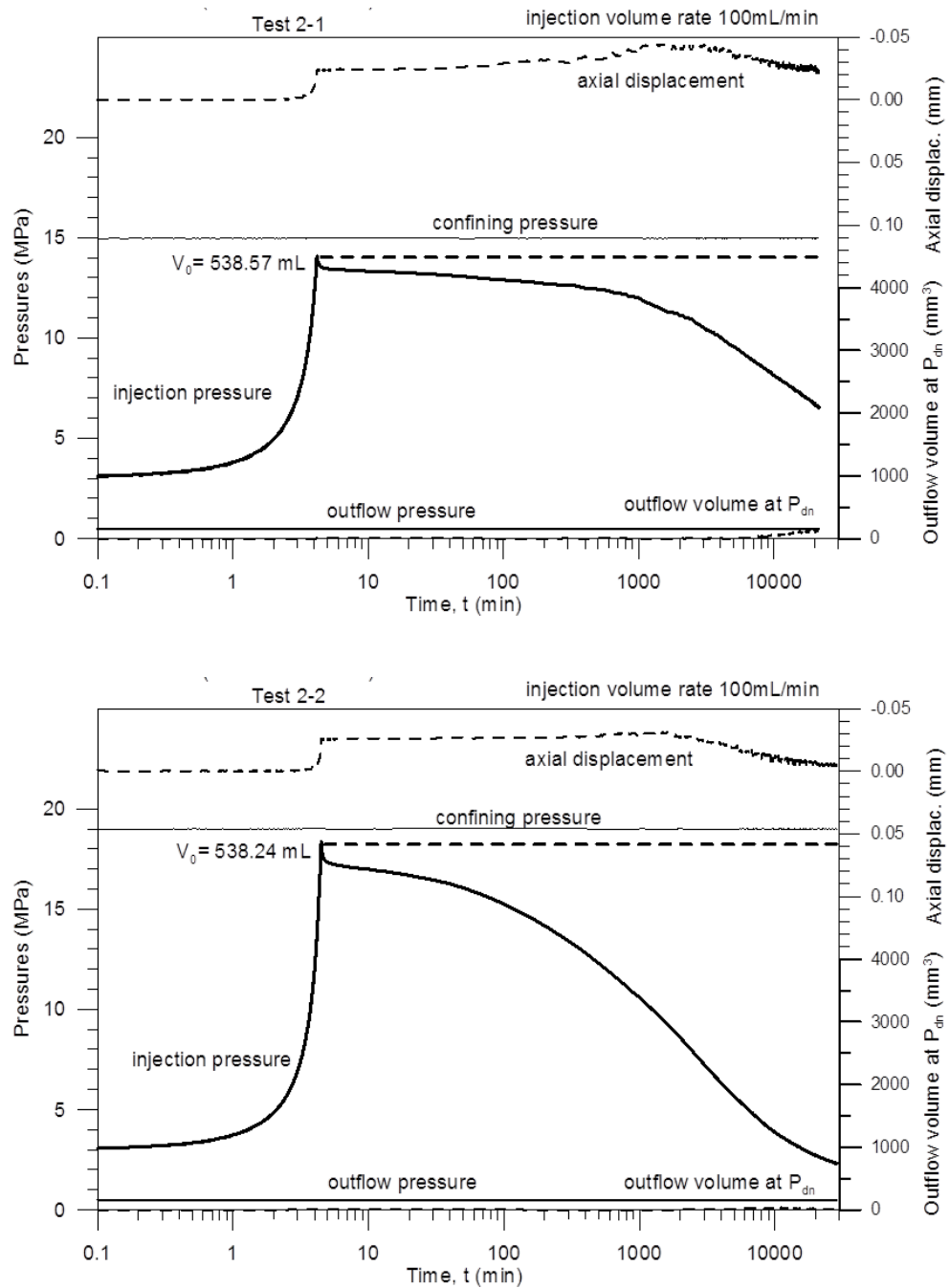


Fig. 3-14: Gas-injection experiments on core sample OED/Opalinus Clay (879.79 – 880.01 m) from the SLA-1 borehole with isostatic stress conditions and flow orthogonal to bedding (from Romero & Gómez 2013)

Measured time evolution of pressures at injection and outflow sides together with outflow volume and axial displacements at confining pressures of (a) $p = 15$ MPa and (b) $p = 19$ MPa.

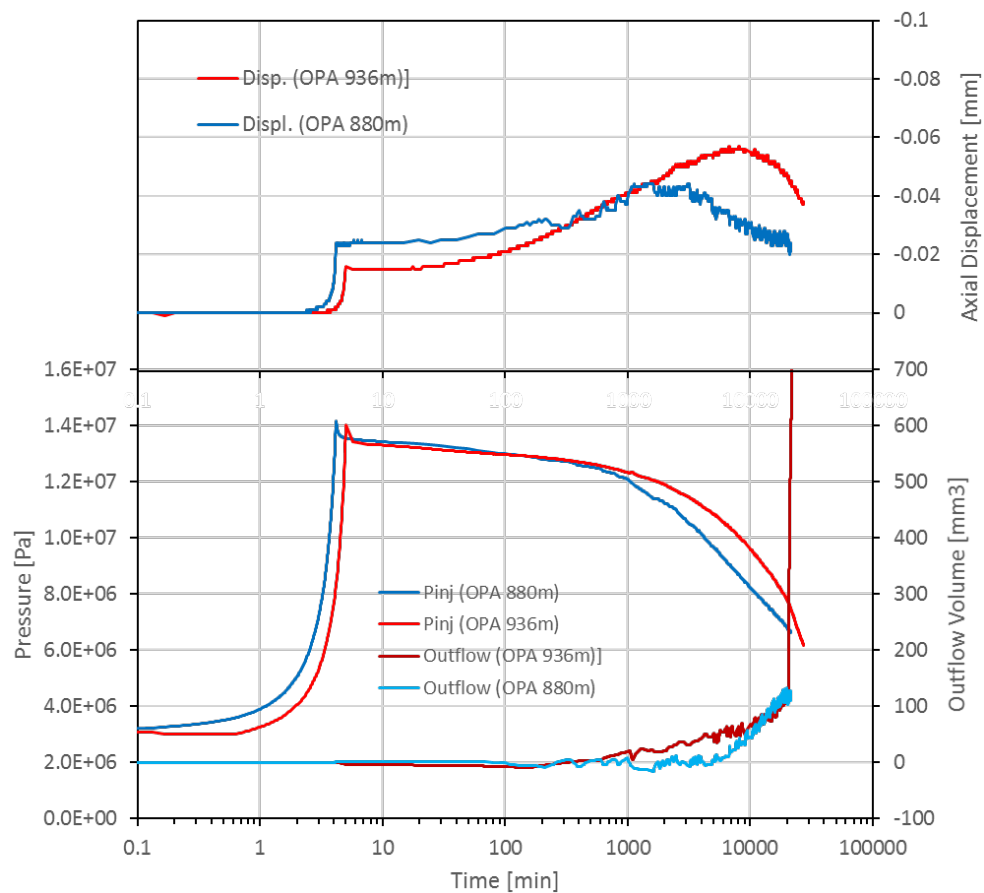


Fig. 3-15: Air-injection test perpendicular to bedding for Opalinus Clay core samples from the Schlattigen SLA-1 borehole at 880 m and 936 m b.g.l., respectively

Measured pressures at the injection side and outflow volumes at the downstream side together with axial displacements (from Romero & Gómez 2013, and Romero & González-Blanco 2015).

The air-injection tests on the deep Opalinus Clay core samples from different depths in the Schlattigen borehole in Switzerland displayed similar responses to those from the Mont Terri borehole (see Section 3.2.5, Fig. 3-26). Only cores perpendicular to bedding were available from the deep borehole. Tests on deep cores showed a later outflow response and a more distinct decline in injection pressure after shut-in (Fig. 3-15). Similar to the shallow analyses, a series of complementary tests performed preceding the air-injection tests, which included compression tests, water-permeability tests and water-retention measurements as well as mercury-intrusion porosimetry before and after the air-injection test. These tests and associated analyses are described in detail in Romero & Gómez (2013) and Romero & González-Blanco (2015). The axial deformation of the deep cores (Fig. 3-15) shows a similar response as those from the shallow cores (see Section, Fig. 3-26). However, the compressibility from the compression tests and the initial porosity are much lower for the deep core samples than for the shallow core samples (see Section 3.2.5, Tab. 3-2 and Tab. 3-3). Potential non-reversible changes in the pore volume were indicated by the measured pore-size distributions before and after the air-injection tests, changing to a bi-modal pore-size distribution with new “pores” whose entrance pore size were higher by two orders of magnitude (Romero & González-Blanco 2015).

A new laboratory programme was initiated as part of the EURAD-GAS project (2020 – 2024). Nagra provided Opalinus Clay core material from the TBO programme, aimed at performing water- and gas-permeability measurements on intact and remoulded Opalinus Clay samples in oedometric configurations. Special focus was on the volumetric behaviour of the Opalinus Clay in response to gas-invasion processes. Tests were conducted at high and low gas-pressure build-up rates, representing undrained and drained gas-injection conditions. A marked dependence of the volumetric behaviour of the Opalinus Clay on the gas-pressure build-up rate was confirmed by Llabjani (2024). Gas-injection tests were carried out on intact Opalinus clay samples in an oedometric cell at two different injection rates, namely 0.2 mL/min and 0.05 mL/min (initial volume in the reservoir $V_0 = 500$ mL). Total vertical stress was 15 MPa and remained constant during the entire test sequence, comprising a constant-rate, gas-injection period, a constant gas-pressure phase (10 MPa) and a constant upstream reservoir volume phase (Fig. 3-16). During the constant-rate gas-injection phase, the gas pressure at the upstream boundary increased from 3 to 10 MPa, remaining 5 MPa below the vertical stress during the entire test sequence.

The mechanical response revealed vertical expansion upon gas pressure build-up, indicating larger vertical expansion for the rapid gas-injection test in the short term. At constant gas pressure, vertical compression and subsequent stabilisation of the strain were observed for the rapid gas-injection tests, whereas the strain remained stable for the slow gas-injection test. In the final test (“constant upstream reservoir volume”), vertical compression was observed both for the rapid and slow gas-injection tests. The hydraulic response displayed a delayed gas breakthrough in the rapid gas injection test. The outflow increased with time until steady state conditions were reached. Once steady state conditions had been reached, no significant differences were observed in the long-term for slow/rapid gas injection tests. In both tests, outflow decreased during the gas dissipation.

The mechanical and hydraulic responses on slow/rapid gas injections exhibit similar characteristics as the gas-injection tests by Gonzalez-Blanco et al. (2022) as part of the EURAD-GAS project (Levasseur et al. 2024). The interpretation of the results in terms of drained / undrained behaviour is consistent with the general deformation behaviour of clayey geomaterials. In the undrained case with rapid gas pressure build-up, it is more likely that gas transfer is associated with larger deformation due to generation of excess porewater pressure during the transient phase. In contrast, in the drained case with slow gas-pressure build-up, gas transfer is less likely to generate excess porewater pressure and smaller deformation was observed accordingly. The final compressive strain observed on both tests could be the result of two phenomena: (i) a higher locally effective stress as a result of remaining suction within the specimen; and (ii) the applied total stress at the bottom of the specimen increased locally due to the applied gas pressure.

The comparison between the slow and rapid gas-injection tests suggests that gas-induced porewater displacement is a key feature during gas-invasion processes in a clay-rich host rock, namely the visco-capillary two-phase flow regime. On the other hand, quantitative analyses using the H²M model have shown an enhanced gas phase mobility in both tests, suggesting the development of preferential flow paths, leading to greater permeability and measured gas flow.

Those observations suggest that similar mechanisms control the hydro-mechanical response of Opalinus Clay during gas-invasion processes in both tests, such as porewater displacement by gas and a change in effective stress that can induce differential deformation in the porous media and the development of preferential pathways as a consequence. In other words, both mechanisms, namely visco-capillary two-phase flow and dilatancy-controlled gas transport, are relevant and necessary to describe the hydro-mechanical response of Opalinus Clay to gas invasion.

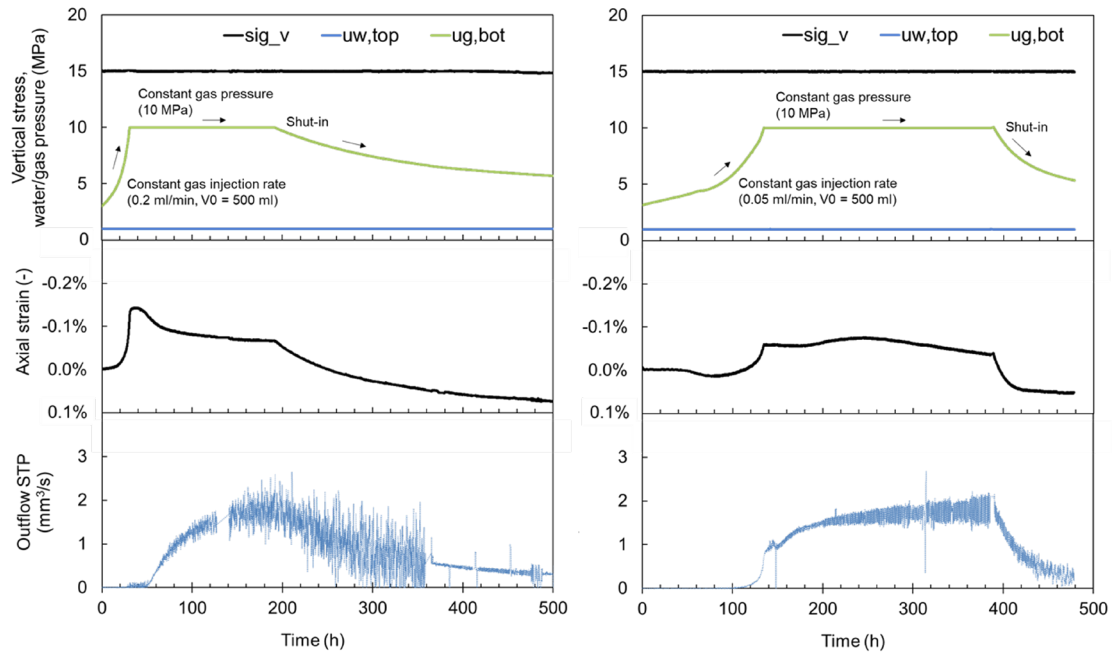


Fig. 3-16: Gas-injection experiments on Opalinus Clay samples in an oedometric cell with gas flow perpendicular to bedding

Transients of liquid / gas pressure and vertical stress (top), average axial strain (centre) and outflow volume (bottom) using controlled volume rates of 0.2 mL/min and 0.05 mL/min (total volume $V_0 = 500$ mL).

3.2.3 Gas-flow behaviour in fault-gouge material

As part of Tasks 3.1 and 3.2 for EURAD-GAS / Marschall et al. (2024), EPFL's experimental programme on Opalinus Clay addressed three major aspects: (i) rock failure initiation and propagation due to gas pressure; (ii) gas transport in remoulded and recompacted Opalinus Clay simulating fault gouge behaviour; and (iii) self-sealing processes after gas invasion. The detailed descriptions of the experimental set-up, material properties of the test samples, and the testing protocol are given in EURAD-GAS / Marschall et al. (2024). The core samples used for the experimental campaign were taken from the deep borehole in Trüllikon (TRU1-1) in the Zürich Nordost siting region (Ammen & Palten 2021) at a depth of about 850 m.

The pore structure of the Opalinus Clay was studied with MIP tests, where a freeze-drying technique was adopted to prepare the samples, accounting for the conformance and compressibility effects of the sample below the entry pressure of mercury (Comisky et al. 2011). The MIP results are shown in Fig. 3-17, in terms of the intruded void ratio and pore-size density function versus pore diameter for the natural Opalinus Clay sample (OPA_848) and the remoulded and recompacted sample (OPA_R14).

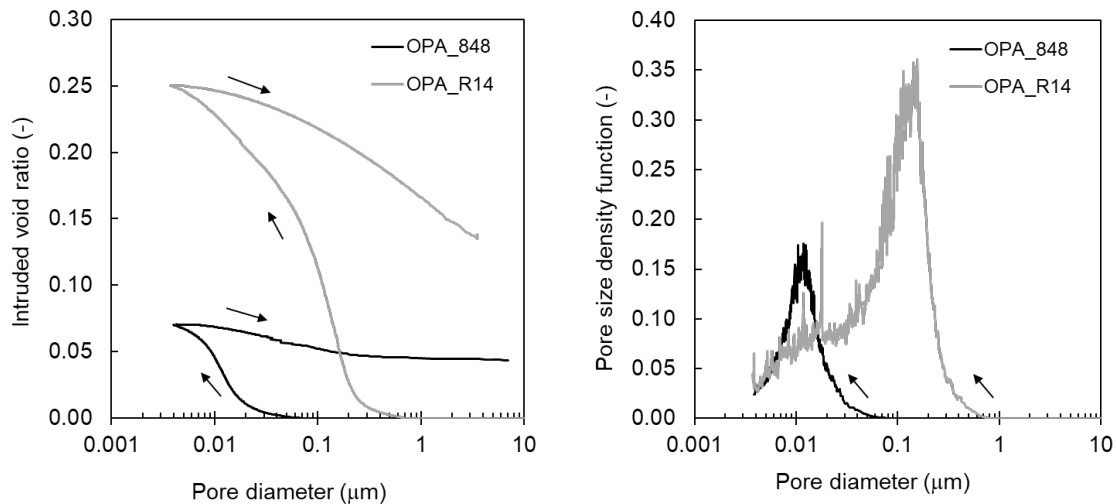


Fig. 3-17: MIP test result: intruded void ratio (left) and pore-size density function (right) for the natural Opalinus Clay sample (OPA_848) and the remoulded and recompacted sample (OPA_14)

A high-pressure oedometer cell applying vertical stress up to 100 MPa and injecting fluids (water, gas) up to 20 MPa and 16 MPa, respectively, were used for the water-retention measurements and the water-/gas-injection tests. The one-dimensional compression made it possible to assess the relationship between deformation, expressed in terms of void ratio, and the applied stress. Additionally, the water permeability was computed based on the one-dimensional consolidation theory for shales (Ferrari et al. 2016). Comparison of the compaction of remoulded Opalinus Clay with respect to natural Opalinus Clay indicated that, at the maximum effective stress level, the void ratio of the remoulded material is still far from that of the intact Opalinus Clay, suggesting that the porosity of the natural Opalinus Clay is related not only to the mechanical compaction and fabric configuration but also to diagenesis (Favero et al. 2016). However, estimated intrinsic water permeability for both natural and remoulded Opalinus Clay indicated a significant decrease with decreasing void ratio upon compaction (Favero et al. 2016).

The water-intrinsic permeability of the natural Opalinus Clay was obtained in the range of $2.7 \times 10^{-21} \text{ m}^2$ (Fig. 3-18a) and is in agreement with values reported in the literature (e.g., Marschall et al. 2005, Crisci et al. 2019, Minardi et al. 2021). In comparison, the remoulded Opalinus Clay showed significantly lower water-intrinsic permeability upon compaction (Fig. 3-18b), and is in agreement with values reported in the literature (Favero et al. 2016). The results for the natural and remoulded Opalinus Clay were fitted according to an exponential law of water permeability values as a function of the void ratio, respectively (Fig. 3-18).

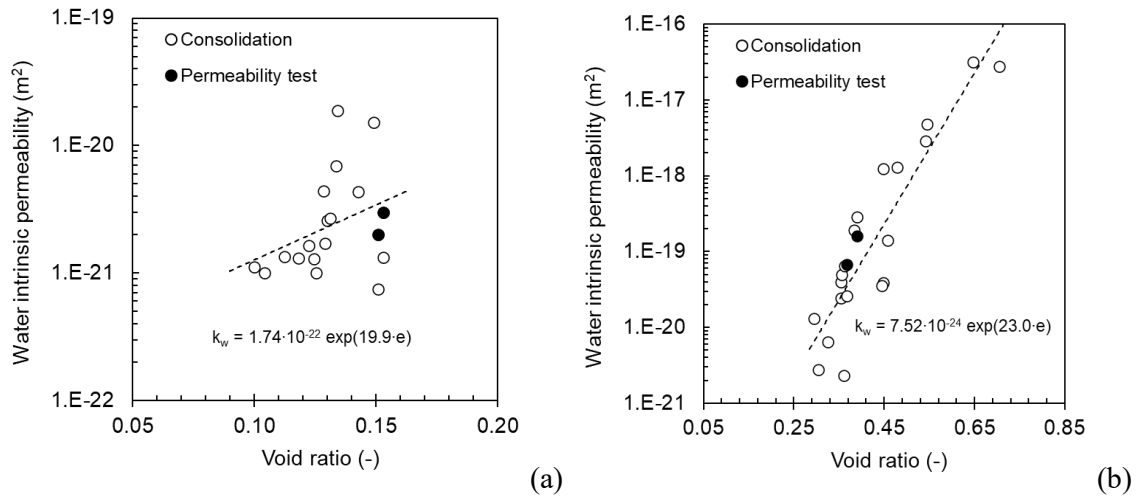


Fig. 3-18: Water-intrinsic permeability of (a) natural Opalinus Clay and (b) remoulded and recompacted Opalinus Clay obtained from constant-head permeability tests and from consolidation analyses

(From Marschall et al. 2024).

The vapour-equilibrium technique (VET) was used for the application of wetting/drying processes and the definition of the water-retention behaviour. Water-retention properties showed coupling between water content and strains. The natural Opalinus Clay (Fig. 3-19) exhibited anisotropic and irreversible behaviour, while the remoulded and recompacted Opalinus Clay (Fig. 3-20) behaved isotropically and reversibly upon suction changes. Larger deformation was observed in the axial direction, as a result of opening/closure of the bedding planes, and irreversible strain was accumulated upon wetting.

Gas-injection results of the natural Opalinus Clay samples indicated both visco-capillary two-phase flow and dilatancy-controlled gas-flow mechanisms, suggesting porewater displacement and changes in effective stress as key features during gas invasion. In the undrained case with rapid gas pressure build-up, it is more likely that gas transfer is associated with larger deformation due to the generation of excess porewater pressure during the transient phase. The comparison between the slow and rapid gas-injection tests suggests that gas-induced porewater displacement is a key feature during gas-invasion processes in a clay-rich host rock, namely the visco-capillary two-phase flow regime. Preliminary analyses showed enhanced gas-phase mobility, indicating the development of preferential flow paths. Comparison of the water-intrinsic permeability and the PSD function before and after gas invasion of natural Opalinus Clay suggested no significant differences, indicating that the barrier function of the host rock is not impaired by the gas-invasion processes. Overall similar results were obtained in similar experiments and analyses on Boom Clay performed by CIMNE as reported in Marschall et al. (2024) and summarised in Section 3.4.3.

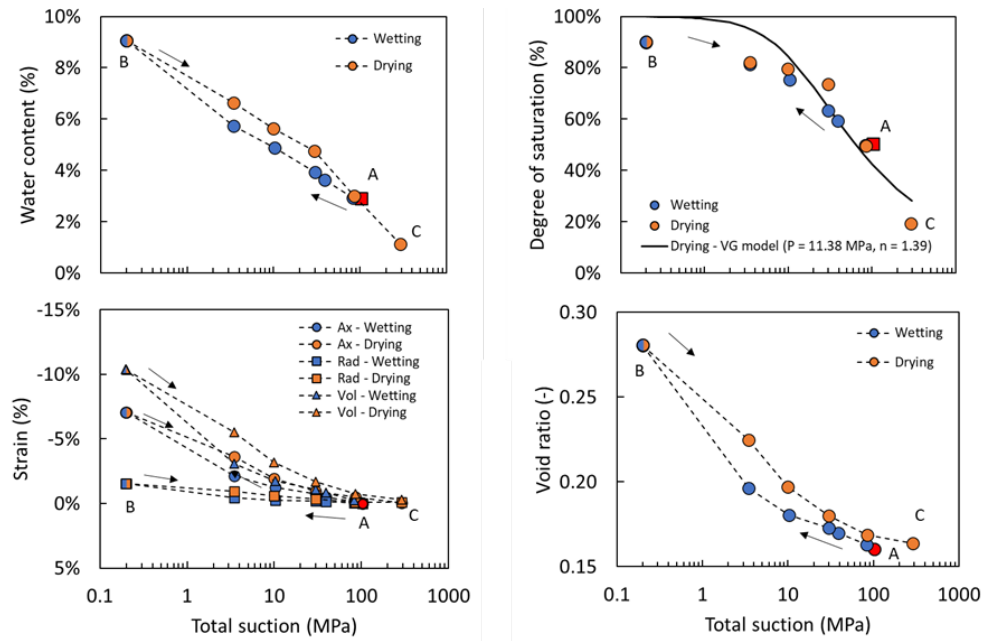


Fig. 3-19: Water-retention behaviour of natural Opalinus Clay (OPA_848): initial wetting and drying paths

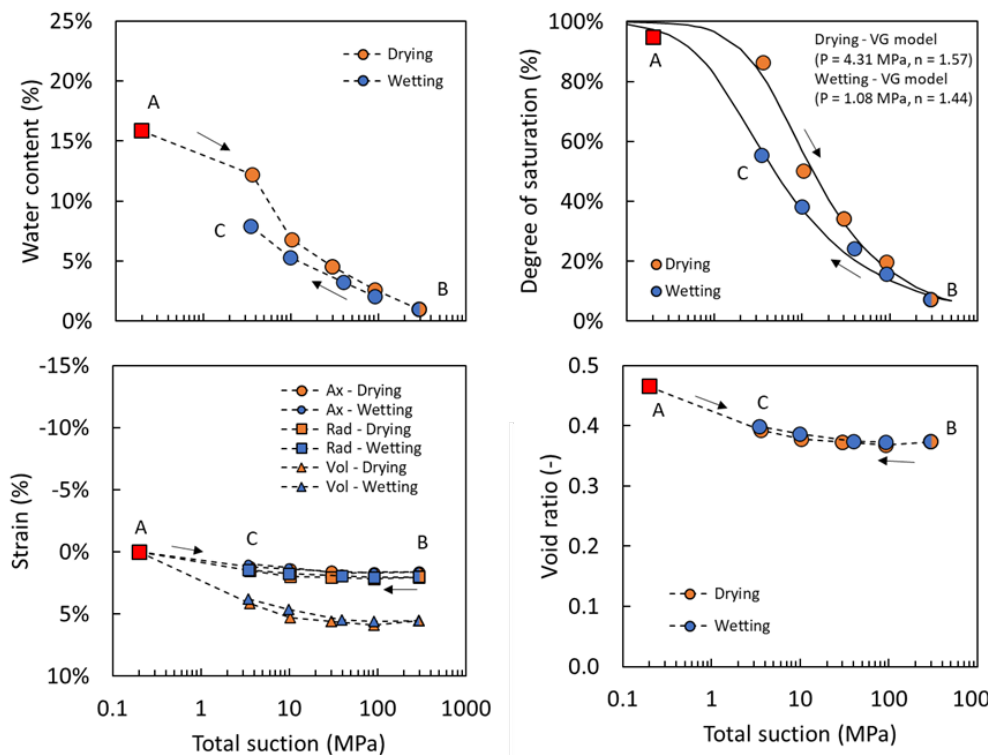


Fig. 3-20: Water-retention behaviour of remoulded and recompacted Opalinus Clay (OPA_R5): drying and wetting paths

3.2.4 Gas-threshold pressure tests as part of the TBO campaign

In Stage 3 of the SGT, dedicated in-situ tests were performed as part of the TBO campaign to investigate the performance of the Opalinus Clay when subjected to high gas pressures. Gas-threshold pressure tests (GTPT) are a special type of packer tests, aimed at determining the gas pressure needed to invade an initially fully saturated porous medium. A total of six GTPTs were performed, namely MAR1-1-OPA3-GTPT, BOZ1-1-OPA4-GTPT, BOZ2-1-OPA4-GTPT, STA2-1-OPA3-GTPT, STA3-1-OPA4-GTPT and RHE1-1-OPA1b-GTPT. Complementary information from drill-core analysis, geophysical logging and laboratory tests on core material is available for an integrated interpretation of the GTPT data. The detailed understanding of fracture initiation and fracture propagation processes together with the site-specific confirmation of the self-sealing potential of the Opalinus Clay will form an important input for performance assessment and consequence analyses as contributions to the general licence application for a deep geological repository in Switzerland.

Fig. 3-21 shows the inferred fracture pressures from the GTPTs in the different boreholes, plotted as a function of depth (midpoint depths of the test interval). They show an overall increase with depth as expected and fall below the lithostatic pressure curve (assuming a bulk density of 2.5 g/cm^3 and a gravitational acceleration $g = 9.81 \text{ m/s}^2$). However, they trend more closely to the 80% lithostatic pressure curve. The 80% lithostatic pressure is typically assumed to be the potential onset of pathway dilation in the deep clay formation (Nagra 2008). Also shown in Fig. 3-21 is the fracture pressure of the GTPT in the COx performed in the Andra borehole EST363 at Bure, which corresponds to the lithostatic pressure at the test-interval depth.

The GTPTs were conducted by means of constant-rate gas-injection phases (GRI), which were typically characterised by a linear pressure increase to a peak pressure followed by a sudden pressure drop at continued gas injection, indicating the fracture opening. The tests in the different boreholes were conducted with different injection rates ranging between 1 NL/min and 5 NL/min. Fig. 3-22 shows the computed downhole gas-flow rates at the test-interval depths in the different boreholes.

For the GTPTs at the TBO boreholes, an outlier is the fracture pressure inferred from STA2-1-OPA3 which, at 12,275 kPa, is much lower than expected at that depth (Fig. 3-21). The GTPT showed a significant pressure response in the bottom (P1) interval during the GRI phase prior to fracturing. Although there is no clear explanation of the observed pressure response in P1, it probably increased the formation pressure and decreased the effective stress, resulting in the lower-than-expected fracture pressure.

BOZ1-1-OPA4 and STA3-1-OPA have fracture pressures of 12,785 kPa and 16,225 kPa (Fig. 3-21), respectively, characterised by narrow peaks with sharp pressure drops leveling off to near-constant pressures during the GRI phases. The other remaining GTPTs have broader peaks followed by a more gradual pressure decline during the GRI phases. The GTPTs in BOZ1-1 and STA2-1 (bold labels in Fig. 3-21 and Fig. 3-22) showed gas bubbles in the tubing during the GRI phases, which indicates some gas leakage, but they follow the same overall trend. BOZ1-1a represents the gas-flow rates after the first fracture subject to an injection rate of 1 NL/min, and BOZ1-1b represents the gas-flow rates after the refracture subject to the higher injection rate of 4 NL/min (Fig. 3-22). The difference in the observed fracture pressures in BOZ1-1 (Fig. 3-21) could be used to estimate a fracture volume of 1.83 L, though it is not clear how the observed gas leakage may have affected the volume estimate. All other GTPTs were done with a single fracture event during the GRI phase, which was followed by a recovery phase (GRIS) after gas injection stopped. The resulting pressure decline during the GRIS phase is typically used to estimate the gas-threshold pressure by the Horner plot extrapolation, indicating the onset of gas migration into the formation, as described below. However, the observed pressure decline can also be used to estimate the downhole gas flow into the formation or fracture.

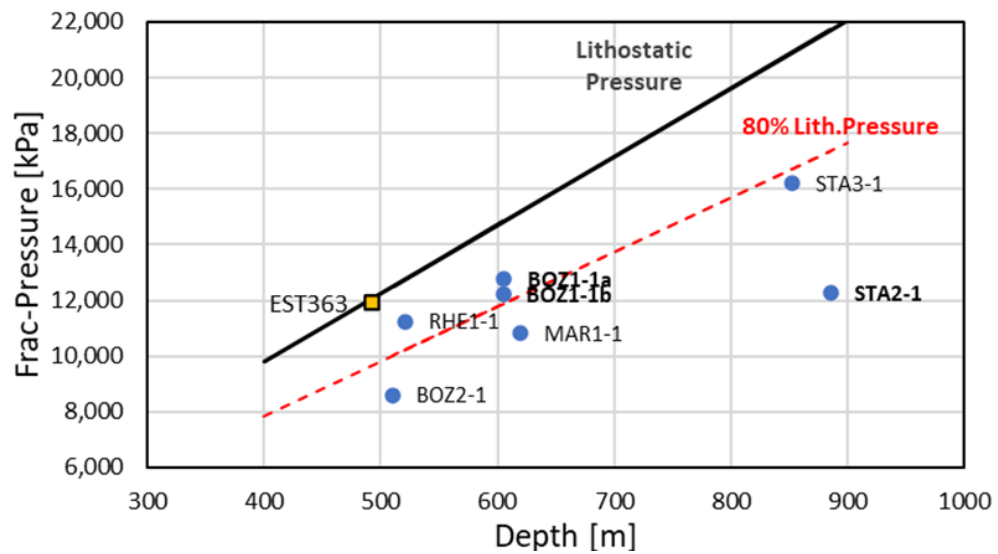


Fig. 3-21: Fracture pressures as a function of depth from the GTPTs in the different boreholes compared to the lithostatic pressure curves

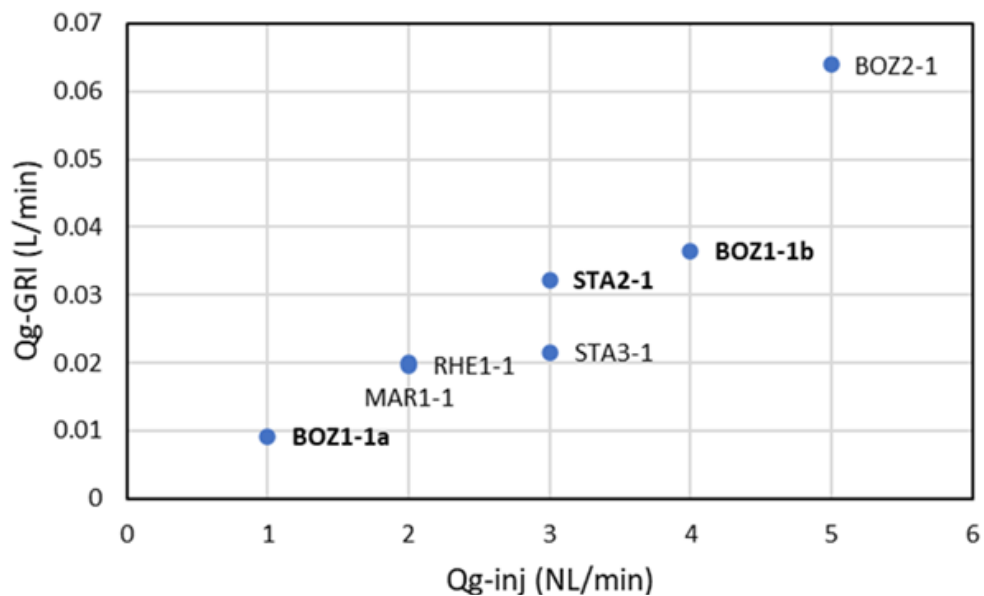


Fig. 3-22: Downhole gas flow rates during the GRI phases after the fracture as a function of the-gas injection rates from the GTPTs in the different boreholes (bold: observed gas bubbles in annulus)

The GTPTs in the different boreholes are preceded by hydrotests with a series of test sequences (typically a PSR followed by a PW or an SW phase) which are used to estimate the transmissivity of the formation over the packer-test interval to determine the hydraulic conductivity of the formation. A few GTPTs were followed by a second hydrotest to compare the estimated hydraulic conductivity before and after the GTPT and to characterise the self-sealing behaviour of the formation.

The relationships between the best-estimate hydraulic conductivities from the hydrotests and the downhole gas-flow rates during the GRI phases after the fracture and the maximum gas-flow rates during the subsequent GRIS phases for the different GTPTs are summarised in Fig. 3-23. The x symbols are the flow rates from the GRI phases and the o symbols are the maximum flow rates during the GRIS phases, both with hydraulic conductivities from the hydrotest prior to the GTPT. The filled symbols (with labels below the symbol) represent the best estimate of hydraulic conductivities from the hydrotests following the GTPT. In the majority of the cases, the downhole gas-flow rates during the GRI phase compare reasonably well with the calculated peak flow rates in the subsequent GRIS phases, considering that the calculated gas-flow rates from the GRIS phase show typically large fluctuations. An exception is MAR1-1, which indicates larger peak downhole flow rates during GRIS than during GRI following the fracture. For BOZ1-1b, the computed maximum gas flow rate during the GRIS3 phase is significantly lower than during the GRI3 phase following the refracture (Fig. 3-23).

Overall, the results indicate little correlation of the gas-flow rates following the fracture and the initial hydraulic conductivities of the formations. Only BOZ2-1 shows a significant increase in hydraulic conductivity based on the hydrotest after the GTPT compared to the calculated post-fracture gas-flow rates during the GRI and GRIS phases. The only other post-GTPT hydrotests are from STA3-1 and RHE1-1, which indicated only small changes in hydraulic conductivities between the hydrotest prior to the GTPT and that following the GTPTs (Fig. 3-23).

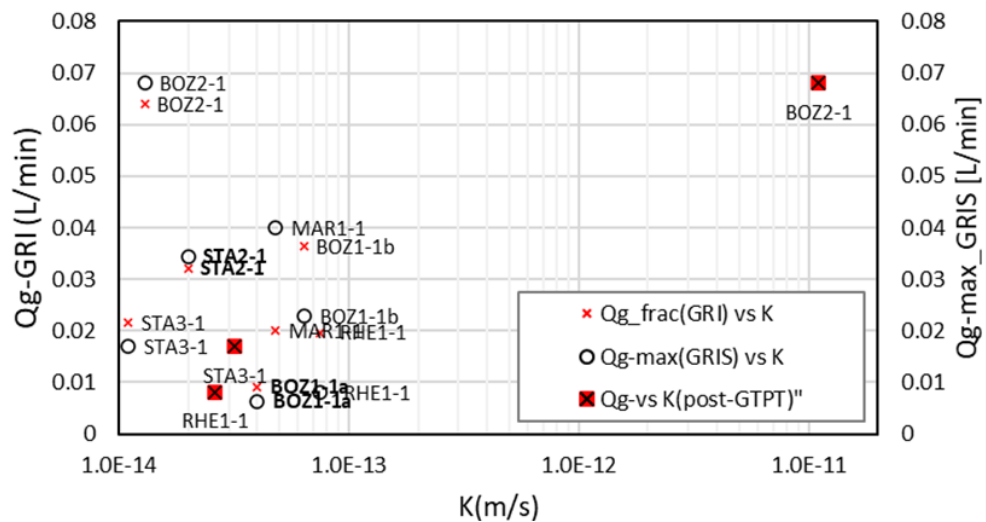


Fig. 3-23: Calculated downhole gas-flow rates during the GRI after the fracture (x symbol) and maximum gas-flow rate during the GRIS phases (o symbol) compared to the best estimate of hydraulic conductivities from hydrotests prior to the GTPTs

The filled symbols represent hydraulic tests after the GTPTs.

The gas-entry pressure can be derived from the gas-threshold pressure, which could be approximated from the Horner-Plot extrapolations of the GRIS phases. This requires a concise estimate of the formation pressure, which is typically determined from the hydrotests preceding the GTPTs. However, those formation pressure estimates were associated with large uncertainties due to the fact that, in these low-permeability environments, it would take an exceedingly long recovery phase to better constrain the formation pressure estimate. Thus, many hydrotests preceding the GTPT yielded unrealistic estimates of formations pressures that indicated hydraulic heads significantly above land surface. As a result, it was assumed that the formation pressures

correspond to the hydrostatic pressures at the GTPT depth interval. The derived gas-entry pressures from the gas-threshold pressure estimated from the Horner-Plot extrapolation of the GRIS phases are plotted as a function of intrinsic permeability using the best estimates of hydraulic conductivities from the hydrotest (Fig. 3-24). In addition, the results from the GTPT in the EST363 borehole at Andra's Bure site are included for comparison.

This GTPT at Bure together with the GTPTs in BOZ1-1 and in STA3-1 fall closest to the Cubic law k - P_{ae} curve (see Eq. 2-27), shown in Fig. 3-24. All other GTPT results are significantly below both the Leverett (Eq. 2-26) and Cubic law curves (Eq. 2-27) and are characterised by broad peaks followed by more gradual pressure declines during the respective GRI phases. The gas-entry pressure values for BOZ2-1 and STA2-1 are very low for the low/permeability estimates and are furthest away from the Cubic and Leverett law curves. As mentioned above, STA2-1 also had a low fracture pressure, which was compromised by the formation pressure increase in the bottom interval. Similarly, the low gas-entry pressure in BOZ2-1 is likely due to the increase in formation pressure resulting from composite borehole model behaviour. However, the hydrotest in BOZ2-1 following the fracture (BOZ2-1b) indicated a more than three orders of magnitude greater permeability than the estimate from the hydrotest prior to the GTPT (Fig. 3-24). In comparison, the hydrotest in STA3-1 after the fracture (STA3-1b) only showed a small increase in the best estimates of hydraulic conductivity compared to STA3-1. The hydrotest in RHE1-1c even indicated a small decrease in permeability compared to the hydrotest prior to the fracture. Both indicate self-sealing behaviour after the fracture, while BOZ2-1b response suggests that the fracture did not completely seal.

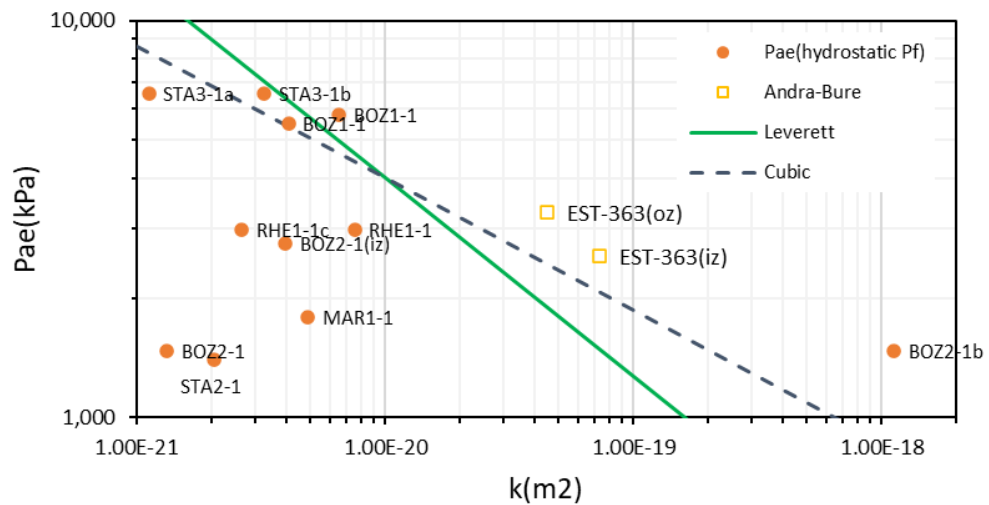


Fig. 3-24: Air-entry pressures versus intrinsic permeability assuming hydrostatic formation pressures at the depths of the GTPTs in the different boreholes compared to the Leverett / Cubic law relationship

3.2.5 Modelling of gas- and water-permeability tests

Back analyses of gas- and water-permeability tests within the framework of Stage 2 of the SGT

Detailed analyses of the gas tests on the shallow samples were conducted by Romero et al. (2012) and Senger et al. (2014b) and for the deep samples by Romero & Gómez (2013), Romero & González-Blanco (2015), and Senger et al. (2018a). For the numerical analyses, a conceptual model for simulating two-phase flow of gas through a low-permeability clay formation was developed and implemented in the numerical two-phase flow simulator TOUGH2. Relevant information from the laboratory experiments in terms of the stress dependence of void ratios and associated changes in permeability were taken into consideration and described in detail in Senger et al. (2014b). These phenomena were implemented in the numerical model by relating the stress dependency through the corresponding effect of pore compressibility on porosity and permeability as a function of pore pressure through the effective stress concept at a fixed total stress.

In TOUGH2, the effect of compressibility is accounted for by the change in porosity ($d\phi$) in response to a change in fluid pressure (dP):

$$d\phi = \phi C_p dP \quad (3-1)$$

The corresponding change in permeability was obtained from the results of the water tests, indicating a log-linear relation between permeability and porosity (Romero et al. 2012), as indicated in Fig. 3-25.

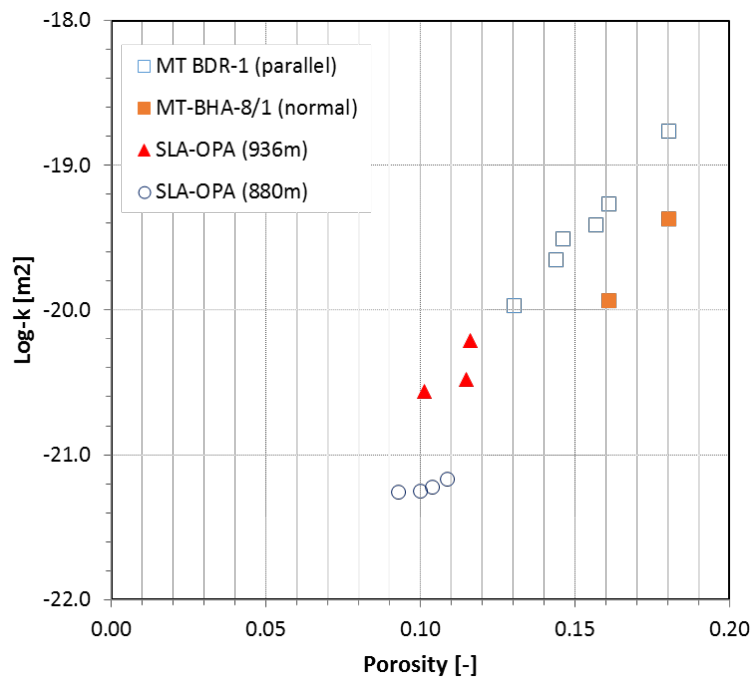


Fig. 3-25: Measured permeabilities and porosities for water tests at different confining stress levels for cores from shallow boreholes (MT) and from the deep borehole (SLA-1) (From Romero et al. 2012, Romero & González-Blanco 2015).

To determine the two-phase flow properties, the laboratory experiments on the water-retention behaviour were used, taking into account the changes in porosity and permeability as well as the corresponding effect on capillary pressure by scaling the capillary strength parameter P_0 with permeability through the Leverett function (Leverett 1941) given in Eq. 2-26.

Only forward simulations were performed using the two-phase parameters based on the measured retention curve data and the estimated permeability from the water test (Tab. 3-2).

Tab. 3-2: Model input parameter (shallow Opalinus Clay / Mont Terri)

	Test 1a (parallel)	Test 1 (normal)
Permeability: $k \text{ (m}^2\text{)}^a$	1.4E-19	4.3E-20
Porosity $[-]^a$	0.20	0.18
Pore compress. $C_p \text{ [1/Pa]}^a$	2.0E-08	1.5E-08
van Genuchten: $P_0 \text{ [Pa]}^b$	18.0E+6	18.0E+6
van Genuchten; n^b	1.67	1.67
Res. water saturation: S_{lr}^c	0.01	0.01
Res. gas saturation: S_{gr}^c	0	0
Initial saturation (S_w) ^c	1	1

^a measured, ^b fitted to WRC, ^c assumed.

The results of the simulations for the air-injection tests parallel and perpendicular to bedding planes are shown in Fig. 3-26. The simulation, incorporated the coupling between the changes in porosity, due to pore compressibility associated with the increased pore-pressure, and the corresponding changes in permeability (Fig. 3-25) and capillary pressure (Eq. 2-26). The simulation results reproduced both the injection pressure response and the outflow pressure response. The peaks of the outflow response are due to the fact that the effect of the release valve at 2 MPa was arbitrarily set at a certain time after the gas-breakthrough response. The injection-pressure response suggests that preferential gas paths were developed as gas migrated into the expanding pores of the samples at increasing injection pressures, resulting in a higher mobility gas behaviour, which, in turn, resulted in a rapid pressure recovery following gas breakthrough.

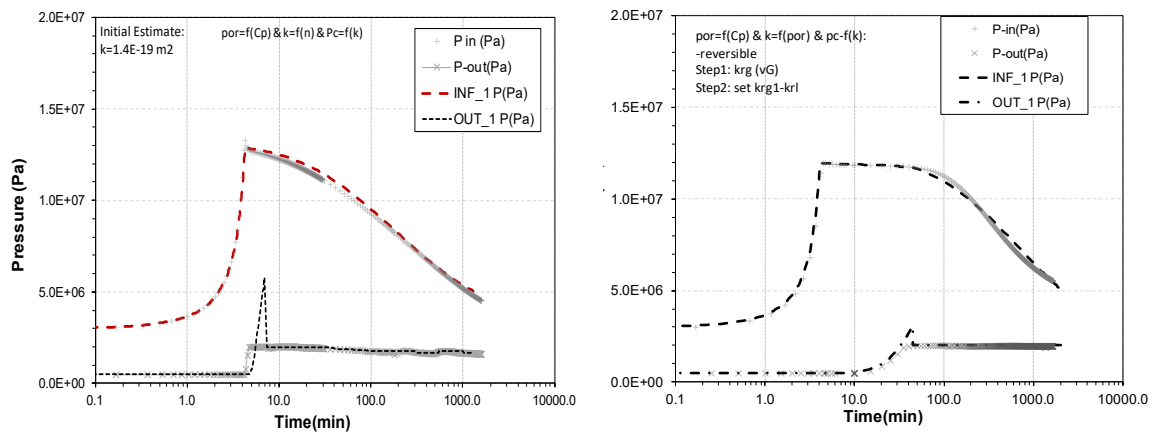


Fig. 3-26: Simulated and measured pressures for air-pulse injection tests on core samples from Mont Terri (“shallow samples”) for flow parallel (left) and perpendicular (right) to bedding

After Senger et al. (2014b).

The air-injection tests on the deep Opalinus Clay core samples (Fig. 3-15) displayed responses similar to those from the shallow samples Fig. 3-26). However, the compressibility from the compression tests and the initial porosity are much lower for the deep core samples than for the shallow core samples (Fig. 3-25). Potential non-reversible changes in the pore volume were indicated by the measured pore-size distributions before and after the air-injection tests, changing to a bi-modal pore-size distribution with new “pores” having an entrance pore size that was greater by two orders of magnitude (Romero & González-Blanco 2015).

Tab. 3-3 summarises the properties of the deep Opalinus Clay core sample, also indicating the higher suction shown in Fig. 3-12 and Fig. 3-13 (Ferrari et al. 2012, Romero & Gómez 2013, Romero & González-Blanco 2015). This information, together with the additional parameters, is used as input for the numerical modelling described in Senger et al. (2018a) and summarised below.

The modelling approach implemented layering, accounting for the non-linear behaviour of soft and stiff layers, and allowing the soft layer to deform more than the stiffer layer, similar to the two-part Hooke’s model described in Liu et al. (2009). The gas-migration front in the axial direction is thus retarded and provides greater storage capacity for the observed gas flow into the sample prior to gas breakthrough.

Tab. 3-3: Model input parameter (deep Opalinus Clay)

	OPA 936 m depth (normal)
Permeability: k (m^2) ^a	3.3×10^{-21}
Porosity: ϕ_r [-] ^a (ϕ_0)	0.1 (0.125)
Pore compress. C_p [$1/\text{Pa}$] ^a	1.0×10^{-9}
van Genuchten: P_0 [MPa] ^b	49
van Genuchten; n ^b	2.05
Res. water saturation: S_{lr} ^c	0.01
Res. gas saturation: S_{gr} ^c	0
Initial saturation (S_w) ^c	1
Coefficient: α [$1/\text{Pa}$] (soft)	1.0 (0.8)
Factor for k - ϕ : c	20
Enhancement factor for k_{rg}	50

^a measured, ^b fitted to wrc, ^c assumed.

The potential changes in hydraulic properties are described as a function of effective stress, using the empirical function given by Rutqvist et al. (2002):

$$\phi = \phi_r + (\phi_0 - \phi_r)e^{-\alpha\sigma'} \quad (3-2)$$

where ϕ_0 is zero effective stress porosity, ϕ_r is the residual porosity at high effective stress, and the exponent α is a rock parameter that is used to represent the “stiff” layer ($\alpha = 1$) and the soft layer ($\alpha < 1$). The exponential function given by Rutqvist et al. (2002) is used to relate the change in porosity to permeability:

$$k = k_0 e^{c(\frac{\phi}{\phi_0} - 1)} \quad (3-3)$$

where k_0 is the initial reference permeability and c is a rock-specific parameter (Tab. 3-3).

In terms of implementation into the TOUGH2 code, the change in porosity is computed from the effective stress, which, in turn, is computed from the simulated pressure and the confining stress:

$$\sigma' = \sigma_T - P \quad (3-4)$$

where the confining stress is constant ($\sigma_T = 15$ MPa), and the pressure represents the gas pressure under two-phase conditions and the liquid pressure under single-phase liquid conditions. The potential impact of two-phase conditions with high capillary suction on the effective stress as described in Nuth & Laloui (2008) was not considered.

The standard TOUGH2 code considers a pressure-dependent permeability to account for the effect of gas slippage through the Klinkenberg function, which describes the change in gas permeability as a function of pressure for a given Klinkenberg parameter b , given as:

$$k_g = k_{g0} \left(1 + \frac{b}{P}\right) \quad (3-5)$$

Instead of the Klinkenberg function, the permeability function (Eq. 2-25) was implemented as a separate option in TOUGH2, whereby both gas and liquid (or intrinsic) permeability can be considered. In addition, the permeability change can be assigned to different directions, allowing for anisotropy in the resulting permeability change. This follows previous approaches for implementing pressure-dependent permeabilities to account for pathway dilation associated with microfracturing in clay material (Senger et al. 2008).

Fig. 3-27 (top) shows the effective stress response computed from the measured injection pressure and the confining stress of 15 MPa. The computed porosity as a function of effective stress assumed a parameter of $\alpha = 0.8$ and 1.0 Pa^{-1} for the “soft” and “stiff” layers (Tab. 3-3). The computed porosity shows a step increase when the peak injection pressure and lowest effective stress are reached (Fig. 3-27: top), which compares to the volume expansion indicated by the steep axial displacement (Fig. 3-26). The observed axial displacement is directly related to the pore volume increase defined by the change in porosity due to the increase in the pressure (Eq. 3-2) and decrease in effective stress (Eq. 3-4).

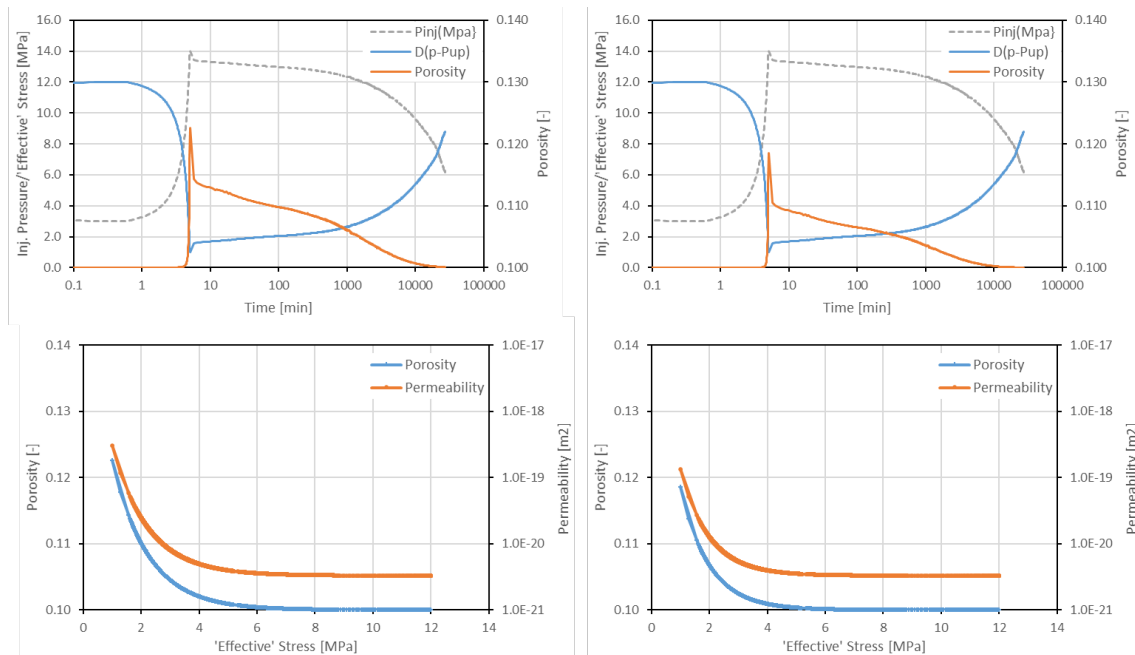


Fig. 3-27: Injection pressure, effective stress and computed porosity for two different values of $\alpha = 0.8$ (left) and $\alpha = 1.0$ (right) based on Eq. 3-2 (top)

The corresponding permeability is based on Eq. 3-3 (bottom), representing the maximum changes at the upstream boundary of the core.

The corresponding change in porosity and permeability as a function of effective stress (Fig. 3-27 bottom) show an exponential increase with decreasing effective stress. The permeability depends largely on the coefficient “c” in Eq. 3-5, which was set to 20 (see Tab. 3-3).

As used in the previous modelling, the change in permeability results in a change in the capillary pressure using the Leverett scale (Eq. 2-26). In addition, a separate enhancement factor for gas permeability is specified, which can be assigned to the different Cartesian directions. With these options, the enhanced gas permeability following breakthrough can be more realistically represented. As described above, the previous modelling of the air-injection test for the shallow core samples oriented normal to bedding required a change in the gas-relative permeability following gas breakthrough to account for higher gas mobility, which was represented by the Grant-relative permeability (Fig. 3-26).

Compared to the previous air-injection tests on the shallow Opalinus Clay cores (Fig. 3-26), the outflow boundary condition was changed. In order to directly simulate the volume increase, a relatively high pore compressibility was assigned to the element representing the outflow chamber. Any mass flow of water and gas into the outflow chamber and corresponding pressure increase are represented by an increase in porosity according to Eq. (3-1), which can be converted to a volume increase for comparison with the measured volume increase of the outflow chamber. The outflow chamber was represented by a single element in the numerical model with a given volume based on the measured volumes of the outlet lines and the initial volume of the outflow chamber reported in Romero & González-Blanco (2015). The change in porosity from an initial value of 1 can be calculated according to Eq. (3-1) based on the pressure increase and a value for the pore compressibility representing the outflow chamber. In order to prevent the pressure in the outflow chamber from increasing significantly, the pore compressibility was calibrated to a large value of $C_p = 1.E-5 \text{ Pa}^{-1}$.

In order to account for some variability in hydraulic properties of the core sample, the core was represented by a two-dimensional vertical cross-section model corresponding to the height (25 mm) and diameter (50 mm). The thickness was adjusted to yield the volume of the core sample. A two-dimensional random heterogeneous permeability field was generated to reproduce the typical variability of the Opalinus Clay (standard deviation of 0.18 m^2), with a geometric average permeability of $3.3E-21 \text{ m}^2$, corresponding to the measured value from the water test at a confining stress of 15 MPa (Tab. 3-2). Because of the relatively small range in measured porosities of the deep core samples (Fig. 3-25), a uniform initial porosity of 0.1 was used for both soft and stiff layers. A highly permeable top layer in the model represents the high-porosity ceramic disc which is connected to a single element representing the outflow chamber. Initial conditions in the core as well as in the outflow line and chamber are fully water-saturated at an absolute pressure of 0.6 MPa. The inflow chamber and inflow lines are air-filled at an initial pressure of 3 MPa, and a constant injection rate of 100 mL/min was applied to the injection chamber by means of a mechanical piston.

For the soft interlayers, the porosity increase was calculated using an α parameter of 0.8 Pa^{-1} , while the parameter for the stiff layers was set to 1.0 Pa^{-1} (Tab. 3-3). The increase in permeability for both layers was for both gas and liquid permeability. In addition, an enhancement factor for the gas/relative permeability was also considered to account for the higher mobility when a gas path has developed, but only parallel to bedding. This represents a permeability increase through microfracturing parallel to bedding which is expected to be air-filled due to the decrease in capillary pressures.

The results for this simulation are shown in Fig. 3-28 in terms of time evolutions of the simulated pressures at the injection chamber and outflow chamber (upper left), air/inflow rates at the bottom of the core, and outflow rates of air and water at the top of the core (lower left), as well the axial displacement (upper right) and outflow volume (lower right). The simulated injection pressures followed the measured pressure during the constant-rate injection phase. However, after the shut-

in, the simulated injection pressures remained nearly constant for about 1,000 minutes when the injection pressure started to decrease with a similar slope as the measured pressure but at a higher pressure level (Fig. 3-28, upper left). The simulated outflow pressure showed only a small increase, which was allowed to compute the porosity increase and corresponding volume increase of the outflow chamber for comparison with the measured outflow volume increase (Fig. 3-28, lower right). The measured outflow volume was converted to an equivalent volumetric rate for comparison with the simulated flow rates of air and water out of the core sample (Fig. 3-28, lower left). In addition, the flow rate of gas into the core sample following the shut-in was estimated from the measured decline in injection pressure, based on the ideal gas law given the remaining volume in the injection chamber. The derived flow rates show relatively large variations due to the variation in the measured pressure responses and are only used for a qualitative comparison with the simulated flow rates.

The simulated flow rate of air into the core sample indicates a steep increase to a peak of about $1.E-7$ kg/s at shut-in followed by a steep decline to about $1.E-9$ kg/s after 100 minutes. Whereas the peak rate compares to the early injection rate into the sample calculated from the pressure decline after the shut-in, the subsequent flow rate significantly underestimated the measured rate. In comparison, the simulated outflow rates show a similar pattern at a later time, whereby the flow rate computed from the outflow volume represents a volumetric rate of the air-water mixture, whereas the simulation shows mass flow rates of air and water (Fig. 3-28, lower right). The computed and measured outflow volumes are in the same range, except at a later time when the computed volumes indicate a steeper increase, which can be related to the greater injection pressures at a later time compared to the measured pressures.

The computed porosity increases of the core sample and corresponding axial displacement reproduce the overall pattern in terms of volume expansion following the shut-in reasonably well; however, the early steep expansion could not be reproduced and the later compression occurs slightly earlier (Fig. 3-28, upper right).

The overall system response is depicted in more detail in Fig. 3-29 and Fig. 3-30 in terms of the spatial distribution of the different variables. Fig. 3-29 shows the simulated porosities, permeabilities and gas saturations after 300 minutes. The simulated porosities (Fig. 3-29, upper left) show the layered pattern with higher porosities in the “soft” layers represented by the value of $\alpha = 0.8 \text{ Pa}^{-1}$ (Tab. 3-2) in accordance with Eq. 3-2. The corresponding permeability increase is shown in terms of “liquid” permeability Fig. 3-29 (upper right) and “gas” permeability in Fig. 3-29 (lower right), indicating the significantly enhanced gas permeability, which is mostly in the horizontal direction, corresponding to microcracks parallel to bedding in the “soft” layers. The vertical extent of the gas-permeability distribution indicates the gas front in the core sample. The resulting gas-saturation distribution shows the increases primarily in the soft layers associated with the increased porosity and large increase in the gas permeability (Fig. 3-29, lower left).

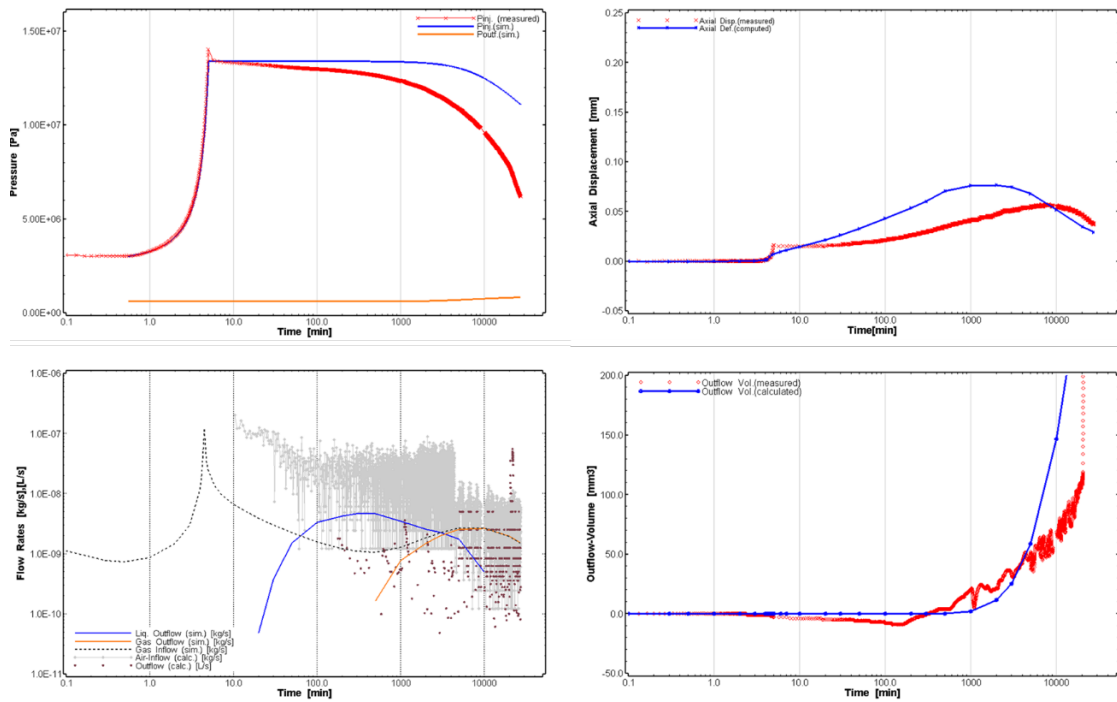


Fig. 3-28: Simulated and measured injection pressures (top left), simulated and measured flow rates (lower left), simulated and measured axial displacement (upper right), and computed outflow volume increase for comparison with measured outflow volume increase (lower right)

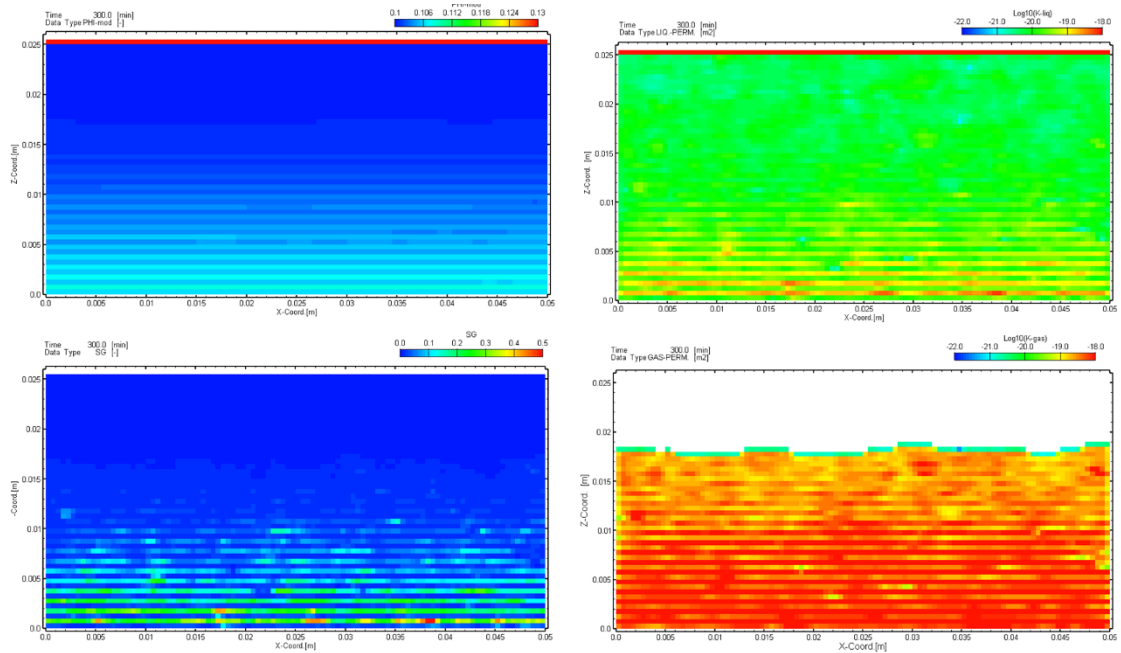


Fig. 3-29: Simulated distribution of porosity (upper left), gas saturation (lower left), liquid permeability (upper right) and gas permeability (lower right) after 300 minutes

The simulation results after 3,000 minutes are shown in Fig. 3-30, with gas saturations and gas pressures at the top and computed gas velocities at the bottom. The gas saturations show the heterogeneous distribution associated with the underlying permeability variation, which was enhanced by the porosity and corresponding permeability increases. The gas saturations in the top layer of the model indicate preferential outflow locations of gas flow. These locations may correspond to the spotted pattern observed at the top surface of the core sample after dismantling (Romero & González-Blanco 2015). The computed gas-flow velocities in terms of magnitude and flow pattern are shown in Fig. 3-30 (bottom). Even though the upward gas pressure gradient is relatively uniform, the gas flow vectors show large variability in direction (Fig. 3-30, lower right).

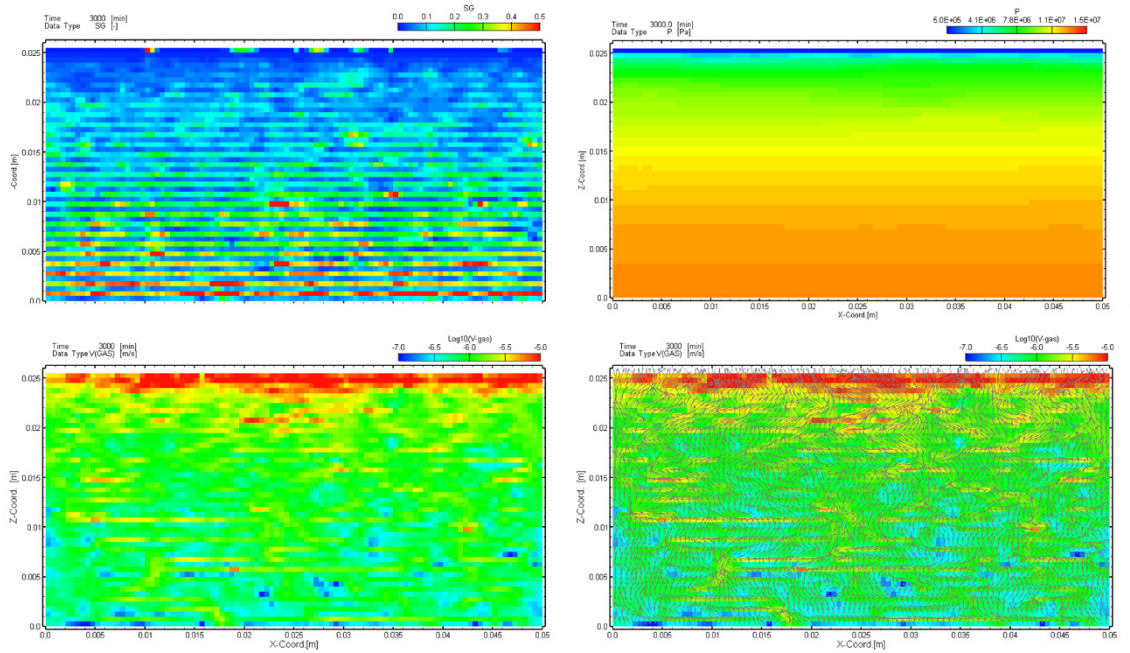


Fig. 3-30: Simulated distribution of gas saturation (upper left), gas pressure (upper right), and gas flow velocities (bottom, with computed gas-flow vectors in lower right) after 3,000 minutes

The implementation of an effective stress-dependent porosity and corresponding permeability change can be used to reproduce the overall pattern of the measured injection pressure and outflow responses as well as the measured axial displacement. It requires representing the bedding of the Opalinus Clay with alternating soft and stiffer materials, allowing for different degrees of changes in porosity and permeability and associated anisotropy, particularly for gas permeability. However, the model could not reproduce the gradual pressure decline following the shut-in and the steep increase in the axial deformation at peak injection pressure.

The measured axial displacement constrains the magnitude of maximum porosity increase, which can be controlled by the α and ϕ_0 parameter in Eq. 3-2. The simulation results used the value $\phi_0 = 0.125$, representing the maximum porosity at zero effective stress. As shown in Fig. 3-27, smaller α values result in a greater increase in porosity. It can be shown that the steep increase in axial displacement can be reproduced by increasing ϕ_0 to 0.15. However, this would significantly overestimate the maximum displacement at a later point in time. The implemented anisotropy in gas permeability is required for the model to reproduce the delay in the outflow response. Romero & González-Blanco (2015) showed some desaturation at the injection surface, suggesting that

some fissures were created in the near surface providing air pathways into the sample. This was indicated by the MIP measurements that were performed on the core samples after dismantling, which showed a significant shift of the water-retention curve to lower saturations compared to the MIP prior to the air-injection test (Romero & González-Blanco 2015). Such fissures perpendicular to bedding near the injection surface could account for enhanced gas flow that would produce a greater pressure decline following shut-in.

Additional analyses within the framework of the EURAD-GAS programme

More recent approaches for modelling the gas-invasion processes in clay involved EPFL's oedometric gas-injection experiments conducted at high/low gas-pressure build-up rates, representing undrained/drained gas-injection conditions (Fig. 3-16). In a first set of analyses, Finsterle et al. (in prep.) implemented Bishop's effective stress model, which is an extension of that described above, where the porosity after Rutqvist et al. (2002) used Bishop's (Nuth & Laloui 2008) effective stress formulation, which includes capillary-pressure effects given as:

$$\sigma' = \sigma_T - P - S_l P_c \quad (3-7)$$

where S_l is the water saturation and P_c the capillary pressure, i.e., porosity is calculated as a function of the initial distribution of fluid pressure, water saturation and total stress. Moreover, pore compressibility is based on the porosity calculated using Eq. 3-2, which is a function of effective stress changes. The potentially enhanced gas permeability is accounted for by the Klinkenberg effect described in Eq. 3-5.

The detailed implementation of the specific gas-injection test is given in Finsterle et al. (in prep.). The calibration of the measured data from the gas-injection tests was conducted using iTOUGH2 with enhancements implemented as described in Finsterle et al. (in prep.). An inversion was performed to match data of (a) pressure at the inlet (bottom of sample), (b) gas-flow rate at the outlet (top of the sample) and (c) axial strain, which is calculated as the integral of the porosity change over the sample length. The residuals were multiplied by an observation-scaling factor, reflecting the relative weight of each data type and making the objective function dimensionless, which is needed for the joint inversion of different data types (Finsterle 2015).

The results of joint inversion of the rapid and slow gas-injection tests described in Finsterle et al. (in prep.) can be summarised as follows: Accounting for capillary pressure effects on porosity changes according to Bishop's model allowed for a qualitative reproduction of the measured axial strains, including a final strain that indicates sample compression beyond the initial state. The inclusion of axial strain data into the inversion slightly increased the mismatch of the model to the pressure and gas-flow rate data, but is considered acceptable given the much-improved prediction of axial strains. On average, the porosity changes inferred from the axial strains are very small and do not lead to noticeable changes in permeability. No significant enhancement of gas permeability in comparison to liquid permeability was derived based on the value of the estimated b parameter in the Klinkenberg equation (Eq. 3-5).

A subsequent approach to simulating EPFL's oedometric gas-injection experiments (Fig. 3-16) implemented the following changes: using the (1) effective stress model after Pereira et al. (2010), and (2) dynamic capillary pressure model after Hassanizadeh et al. (2002).

Pereira et al. (2010) proposed a generalisation of Bishop's effective stress model, which distinguishes between two classes of pores: macropores (with water movement governed by capillary forces) and micropores (with water strongly attached to the solid through physico-chemical interactions).

Therefore, it is assumed that with S_r^m being the saturation of essentially immobile liquid in the micropores, only the effective saturation, given by:

$$S_r^e = \frac{S_l - S_r^m}{1 - S_r^m} \quad (3-8)$$

contributes to effective stress changes in Bishop's equation:

$$\sigma' = (\sigma_T - P) - (\chi \cdot P_c) \quad (3-9)$$

where:

$$\chi = S_r^e + \frac{1}{n} \ln(1 + \exp(-n \cdot S_r^e)) \quad (3-10)$$

The factor χ weighs contributions of the gas pressure P_g and the liquid pressure P_l (through the negative capillary pressure $P_c = P_l - P_g$) to the effective stress in Eq. (3-9). The parameter n is used for exponential smoothing of the effective saturation S_r^e as the liquid saturation S_l approaches S_r^m .

The effective stress model of Pereira et al. (2010) was implemented into iTOUGH2. In addition to the parameters of the classical Bishop model (ϕ_0 , ϕ_r and α), the new parameters S_r^m and n were also treated as adjustable parameters and can be estimated in an iTOUGH2 inversion.

In the dynamic capillary pressure model after Hassanizadeh et al. (2002), the capillary pressure curve depends on the rate of saturation change. Capillary-saturation relationships are typically obtained experimentally under equilibrium conditions. However, if equilibrium between the wetting and non-wetting phase pressures is not reached within a given time, the dynamic effect can be approximated (on a macroscopic level) by the following equation (Hassanizadeh et al. 2002):

$$P_c^{dyn} = P_c^{equ} - \tau \frac{\partial S_l}{\partial t} \quad (3-11)$$

Here, τ [Pa×s] is a material parameter (but may also depend on saturation) that can be interpreted as a capillary damping coefficient, i.e., a measure of the speed with which a change in saturation takes place, with small values indicating rapid equilibration of the capillary pressure. For porous media of low permeability, where the dynamic capillary pressure effect may be relevant, large τ values can be expected. In this simplified model, τ is considered to be non-hysteretic and independent of saturation.

The dynamic capillary pressure model of Eq. 3-11 was implemented into iTOUGH2, with τ as an additional adjustable parameter that can be considered unknown or uncertain and estimated by inverse modelling.

Joint inversions were performed for models where effective stresses are calculated using either the classic Bishop or the Pereira constitutive equations, and using either static or dynamic capillary pressures. All available data (i.e., inlet pressures, outlet gas-flow rates and axial strains from the rapid and slow gas-injection experiments) were jointly inverted to arrive at a single

parameter set for both experiments. If Pereira et al. (2010) is used to calculate effective stresses, the liquid saturation in the micropores, S_r^m is added to the reference set of adjustable parameters; if dynamic capillary pressures are considered, the capillary damping coefficient τ is also added.

Fig. 3-31 visualises the matches obtained after calibration. All four models appear to match all datasets similarly well. However, all models fail to capture the time of gas breakthrough, specifically underpredicting the time for the rapid gas-injection experiment. The axial strain for the slow experiment also has significant, systematic deviations; it is unlikely that they can be reproduced using the simplified inclusion of coupled hydrologic-mechanical effects in this model, which is basically a hydrological model without a formal stress-strain calculation.

Tab. 3-4 shows the parameter estimates for each of the calibrated models. None of the differences in the estimated parameters are significant, indicating that these estimates are relatively robust and not unduly dependent on the details of the mechanical model or the highly transient nature of a laboratory experiment (gas-release processes in a repository are considerably slower, making the inclusion of dynamic capillary pressure effects most likely unnecessary).

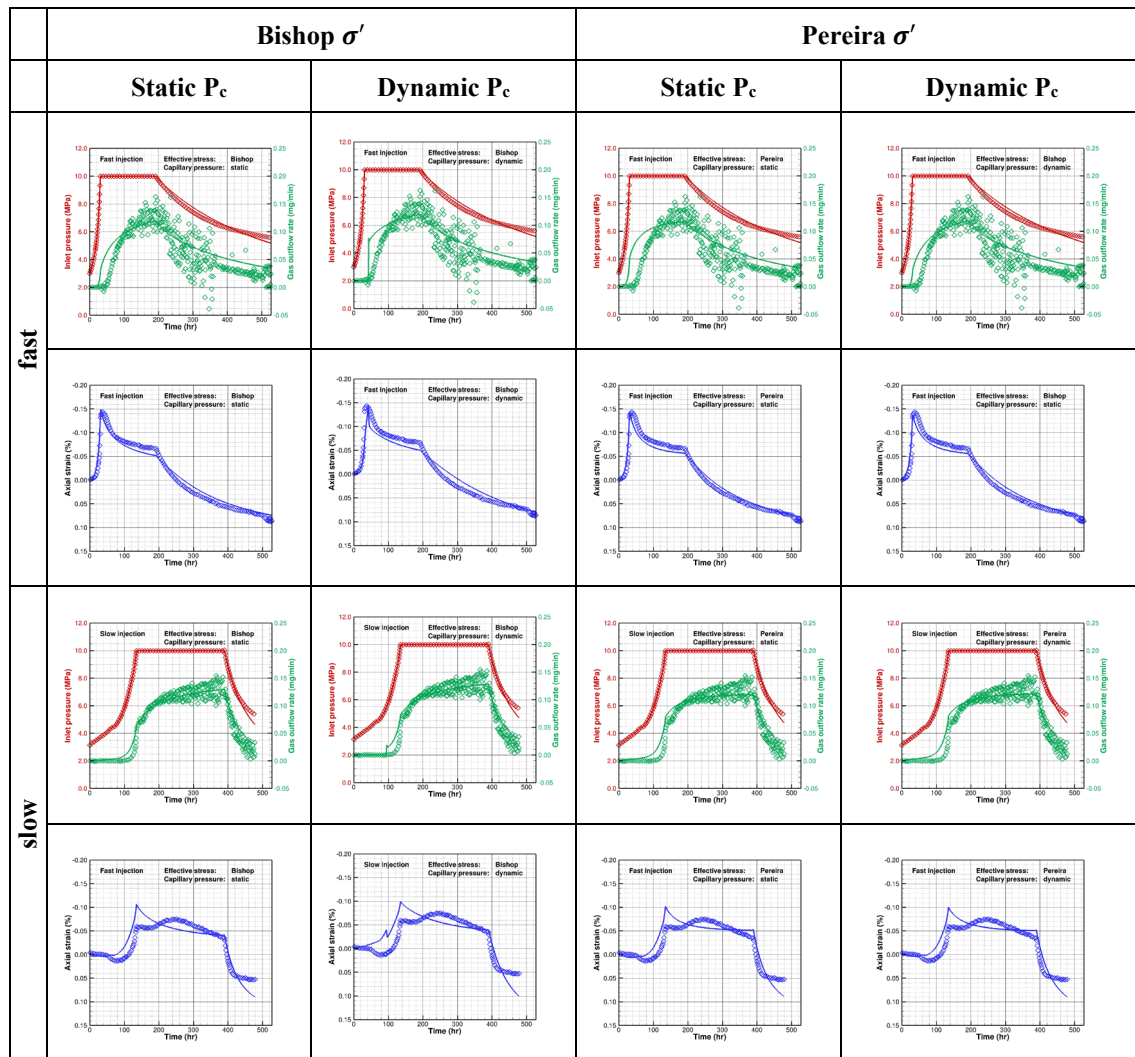


Fig. 3-31: Measured (symbols) and simulated (lines) inlet pressures (red), outlet gas flow rates (green), axial strain (blue) after joint calibration of data from rapid and slow gas-injection experiments for different representations of saturation-dependent effective stress and for static and dynamic capillary pressures

Tab. 3-4: Estimated model parameters from joint inversion of all data from rapid and slow gas-injection experiments for different representations of saturation-dependent effective stress and for static and dynamic capillary pressures

Parameter	Unit	Bishop σ'		Pereira σ'	
		Static P_c	Dynamic P_c	Static P_c	Dynamic P_c
Absolute permeability, k	$\log(\text{m}^2)$ m^2	-20.17 6.8×10^{-21}	-20.29 5.1×10^{-21}	-20.20 6.3×10^{-21}	-20.23 5.8×10^{-21}
Zero stress porosity, ϕ_0	%	14.0	14.3	14.0	14.1
Residual porosity, ϕ_r	%	13.7	14.0	13.8	13.8
Stiffness, β	MPa^{-1}	0.19	0.02	0.15	0.14
Irreducible gas saturation, S_{gr}	$\log(-)$ %	-5.00 LB 0.0	-2.00 1.0	-2.64 0.2	-5.00 LB 0.0
van Genuchten parameter ξ	-	0.44	0.39	0.42	0.40
van Genuchten parameter n	-	1.96	1.42	1.43	1.38
van Genuchten parameter $1/\alpha$	$\log(\text{Pa})$ Pa	6.87 7.4×10^6	6.87 7.4×10^6	7.02 1.1×10^7	7.02 1.1×10^7
Saturation in micropores, S_r^m	-	n/a	n/a	0.65	0.58
Capillary damping factor, τ	$\log(\text{Pa}\cdot\text{s})$ $\text{Pa}\cdot\text{s}$	n/a	12.17 1.5×10^{12}	n/a	12.43 2.7×10^{12}

LB: Parameter estimate is at its specified lower bound.

3.2.6 Reference parameters of the Opalinus Clay

Flow and transport processes in the Opalinus Clay are largely linked to the connectivity of the microscopic pore network of the rock matrix. Fractures tend to self-seal when the effective normal stress (mean normal stress minus pore pressure) exceeds the magnitude of the swelling pressure of the rock. Consequently, it can be assumed that gas transport in the Opalinus Clay occurs mainly in the intact rock matrix as long as the gas pressures are significantly lower than the confining rock stress. The subsequent reference parameters of the Opalinus Clay refer to the gas transport parameters of the intact rock matrix.

Representative hydraulic databases were compiled as part of Stage 2 of the SGT (Nagra 2014a) and complemented in Stage 3 as part of the TBO site investigation programme (Nagra 2024b). The corresponding hydraulic reference parameters have been derived for the host rock and the confining geological units in the potential siting regions (Nagra 2024a). The hydraulic reference parameters form the key input for the derivation of representative two-phase flow parameters. The reference parameters are the same in the three siting regions; reference values and alternative values of the representative two-phase flow parameters of the Opalinus Clay are summarised in Tab. 3-5. Graphical representations of the corresponding capillary pressure and relative permeability curves are given in Fig. 3-32. The capillary strength parameter P_o is scaled via Leverett scaling to the permeability ratio based on a value of $P_o = 34 \text{ MPa}$ and a $k_{\text{ref}} = 2 \times 10^{-21} \text{ m}^2$. The resulting RV for P_o for the RV of $k_i = 1 \times 10^{-21} \text{ m}^2$ is 48 MPa and the corresponding AV of P_o is 15 MPa based on an AV for $k_i = 1 \times 10^{-20} \text{ m}^2$. The RV value for P_o is considered conservatively low with respect to the potential gas pressure buildup and not necessarily supported by empirical permeability – entry pressure relationships. Thus, it follows the safety oriented and conservative approach implemented in the PA.

THM-related properties of the Opalinus Clay are required to assess the impact of heat in the HLW near-field. Thermal and mechanical properties of the Opalinus Clay are summarised in Tab. 3-7.

Tab. 3-5: Reference values for the gas-related parameters of the undisturbed Opalinus Clay for a deep geological repository in Northern Switzerland

Parameter	RV	AV	Remarks
Opalinus Clay			
Intrinsic permeability normal to bedding $k_{\perp}$ [m ²]	1×10^{-21}	1×10^{-20}	RV: Best estimate value from Nagra (2024b). AV: Upper bound value from Nagra (2024b).
Capillary pressure-saturation relationship			van Genuchten parametric model
Capillary strength P_o [MPa]	$P_{o,i}[\text{MPa}] = 34 \sqrt{\frac{k_{ref}}{k_i}}$		Lewerett scaling, based on previous capillary pressure measurements: $k_{ref} = 2\text{E-}21 \text{ m}^2$ Default value $T_0 = 20 \text{ }^{\circ}\text{C}$ for temperature scaling. Residual water saturation $S_{wr} = 0.01$
Shape parameter n	1.67	1.54	RV: derived from capillary pressure measurements (drying path). AV: derived from capillary pressure measurements (wetting path).
Relative permeability-saturation relationship			van Genuchten/Mualem parametric model using the shape parameter n from the capillary pressure curve.
Residual water saturation S_{wr} [-]	0.5	0.1	RV: according to the results of adsorption / desorption measurements, suggesting that 50% of the total pore space can be classified as micro- and mesopores. AV: assuming that most of the porewater is mobile (not supported by experimental data).
Residual gas saturation S_{gr} [-]	0.00	0.003	RV: effective gas-entry pressure of the rock is infinitesimal. AV: the residual gas saturation determines the effective gas-entry value. Effective gas entry values were determined by gas permeability testing at Mont Terri and Benken.
Total porosity [%]	12%	10%	RV: corresponds to the reference value for the porosity in Northern Switzerland. AV: previous porosity values in ZNO.

RV – reference value, AV – alternative value.

Relationship between intrinsic permeability and hydraulic conductivity:

$$k \left[\text{m}^2 \right] = \frac{\eta_w}{\rho_w \cdot g} \cdot K \approx 1 \times 10^{-7} \cdot K \left[\text{m} / \text{s} \right] \text{ for } T = 20^{\circ}\text{C}$$

η_w dynamic viscosity of water [Pa·s]

ρ_w density of water [kg m⁻³]

g gravitational acceleration [m s⁻²]

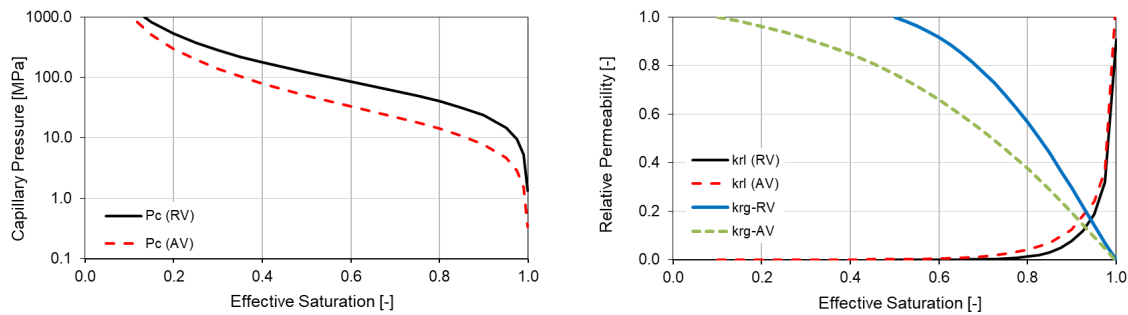


Fig. 3-32: Parametric models of capillary pressure $p_c(S_{eff})$ and relative permeability $k_r(S_{eff})$ for water (w) and gas (g), representative for the Opalinus Clay formation in the three siting regions

RV = reference parameter values and AV = alternative values.

Tab. 3-6: Best-fitting parameters for the van Genuchten model for natural Opalinus Clay and remoulded / recompacted Opalinus Clay

From EURAD-GAS / Marschall et al. (2024).

Suction path	Drying		Wetting	
Specimen	P (MPa)	n (-)	P (MPa)	n (-)
OPA_R848 (natural)	11.38	1.39		
OPA_R5 (remoulded)	4.31	1.57	1.08	1.44
OPA_R14 (remoulded)	6.10	1.51	2.93	1.44
OPA_R50 (remoulded)	7.27	1.52	1.68	1.38

As part of Tasks 3.1 and 3.2 of EURAD-GAS project / Marschall et al. (2024), EPFL's experimental programme on Opalinus Clay addressed, among other aspects, gas transport in remoulded and recompacted Opalinus Clay representative of fault gouge behaviour. The results in terms of the water-intrinsic permeability and water-retention behaviour of remoulded and recompacted Opalinus Clay samples compared to the natural Opalinus Clay sample from the deep borehole in Trüllikon (TRU1-1) in the Zürich Nordost siting region are summarised in Tab. 3-6.

THM-related properties of the Opalinus Clay are required to assess the impact of heat in the HLW near-field. Thermal and mechanical properties of the Opalinus Clay are mainly based on Gaus et al. (2014a) and summarised in Tab. 3-7.

Tab. 3-7: Thermal and mechanical properties for the Opalinus Clay
(From Gaus et al. 2014a).

	Unit	Opalinus Clay	EDZ	Comment
<i>Thermal parameters</i>				
Density - Bulk - Grain	ρ [kg/m ³]	2,450 2,700 ¹	2,450 2,700 ¹	From Nagra (2024a). ¹ Input parameter for TOUGH simulations.
Specific heat	C _r [J/kg K]	995.0	995.0	Values used in this study.
Thermal conduct. - Parallel¹ - Perpendicular¹ - Dry² - Saturated²	T _c [W/m K]	2.8 1.6 1.36 2.1	2.4 1.2 1.36 1.7	Note: the EDZ values are derived from Seiphoori (2022). Seiphoori (2022) – “Thermal conductivity of shallow Opalinus Clay (BCI-21B)”. ¹ Seiphoori (2022), Vomvoris et al. (1992). ² Harmonic mean.
- Therm. expansion grain - Rock framework - Water	T _x [1/ K]	1.5E-6 1.7E-5 ¹ 3.4E-4	1.5E-6 1.7E-5 ¹ 3.4E-4	Wileveau & Rothfuchs (2007). ¹ Input parameter for TOUGH simulations: rock framework.
<i>Rock compressibility</i>				
- Young’s Modulus - Poisson ratio - Porosity	E [MPa] ν [-] ϕ [-]	6,500 ¹ 0.23 ¹ 0.10	3,900 ² 0.115 ² 0.14	¹ Nagra (2024a): derived from bulk modulus – best estimate (drained). ² Nagra (2024a): derived from bulk modulus – minimum (drained). ^{1,2} Nagra (2024a): average perpendicular and parallel to bedding.
Compressibility: $\alpha = 3(1-2 \nu)/E$	α [1/ Pa]	2.5E-10	5.9E-10	Computed from E-modulus.
Pore compressibility: C _p = α/ϕ	C _p [1/ Pa]	2.1E-09	4.2E-09	Input parameter for TOUGH simulations.

3.3 Clay-rich and sandy-calcareous sequences in the confining geological units

3.3.1 Basic geological characteristics of the clay-rich confining geological units

The Dogger above and the Lias/Keuper below the Opalinus Clay are also clay-dominated but include heterogeneities such as Fe-rich oolites, sandy lithologies or limestones (Fig. 3-33). The rocks range from claystones to calcareous marls. In Stage 2 of the SGT, the suite of predominantly clay-rich rock units stratigraphically located between the Opalinus Clay and the Malm was termed «Brauner Dogger». The clay-rich sequences are characterised by similar barrier properties as the Opalinus Clay.

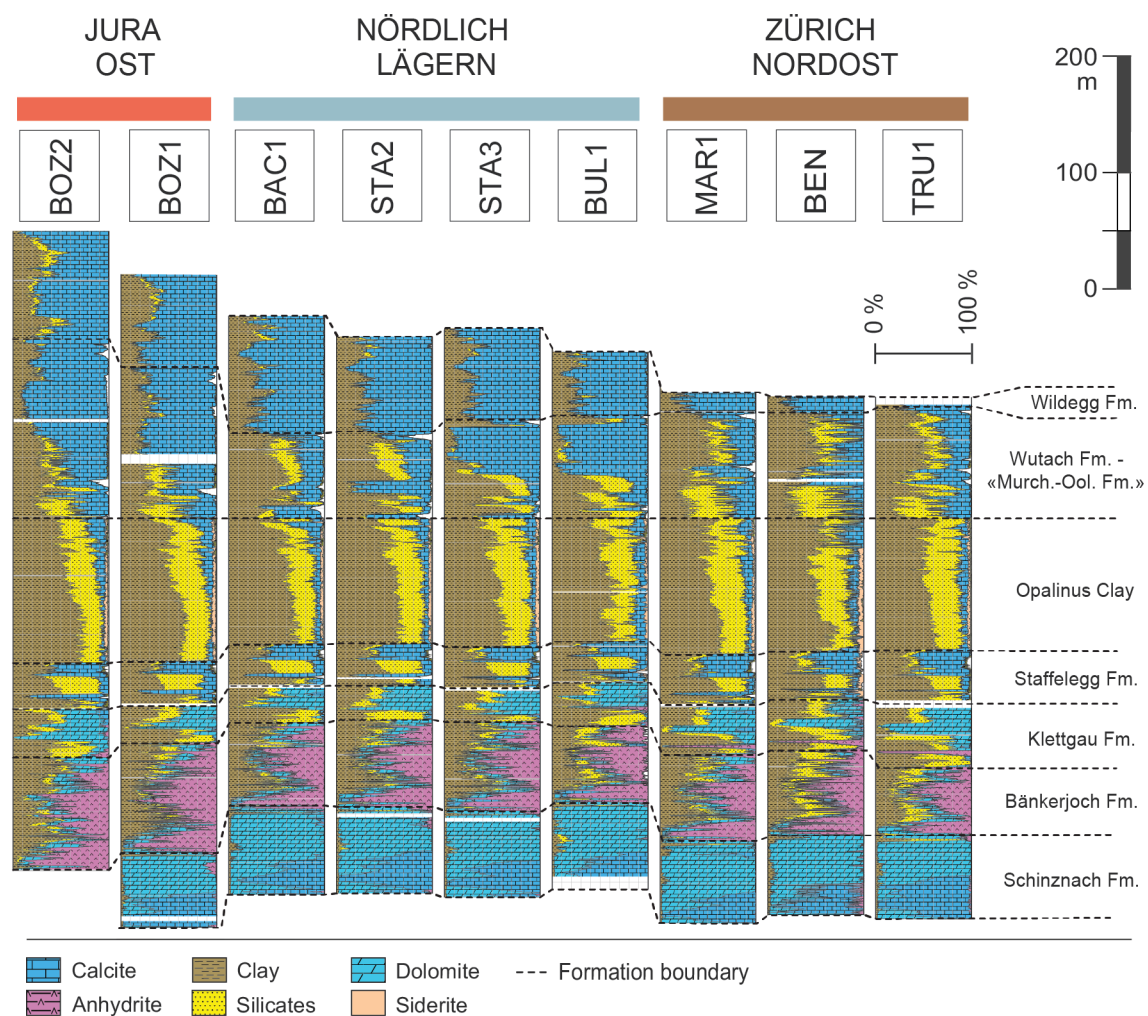


Fig. 3-33: Mineralogical composition of boreholes based on stochastic multiminerall log interpretation

(From Nagra 2024b).

The porosity profiles of the Mesozoic layer stack in the three siting regions are presented in Fig. 3-2. It is obvious that the sequences above and below the Opalinus Clay exhibit a significantly higher variation in porosity. The increased variability of porosity in the Dogger above the Opalinus Clay reflects the higher lithological heterogeneity of this sequence in both the vertical and lateral dimensions. Particularly low-matrix porosities are found in the limestones of the «Herrenwis Unit» and in the Hauptrogenstein. Nevertheless, the average porosity is relatively high (0.10), given the generally clay-rich lithologies present in the upper confining geological units. Porosity in the Staffelegg Formation also varies over a wide range, but the variability shows a systematic vertical pattern over the whole region, reflecting clay content. The lowest porosity values are found in the limestones of the Beggingen and GBR (Grünschholz, Breitenmatt + Rickenbach) Members, whereas all other members yield averages of 0.08 – 0.11.

Further geotechnical characteristics of the clay-rich sequences have been determined as part of recent laboratory programmes, revealing similar stiffness as the Opalinus Clay (Young's modulus in the range of 5 – 15 GPa), but higher strength (UCS values of the intact rock matrix between 30 and 70 MPa) and lower swelling pressures (0.2 – 1 MPa).

A comprehensive database has been compiled in Nagra (2024b), comprising laboratory tests on drill-core samples (on a cm – dm scale) and in-situ hydraulic packer tests (on a m – dm scale). Hydraulic tests on drill-core samples have the advantage that the matrix properties can be related to a well characterisable sample, e.g., in terms of mineralogy or porosity. The matrix hydraulic conductivities, perpendicular to bedding, scatter in a narrow range around 10^{-13} m/s (Fig. 3-34). There is no obvious correlation with mineralogy and porosity. Given the substantial lithological variability, this can be taken as another indication that diagenetic cementation of clay-poor samples is the cause for the low hydraulic conductivities. Similar trends are observed by in-depth interpretation of in-situ tests, e.g., a negative correlation of hydraulic conductivity with carbonate content in the Passwang Formation in JO and the Wedelsandstein Formation in ZNO and NL.

A major effort was invested in in-situ tests for the hydraulic characterisation of the confining geological units. The investigations in the clay-rich sequences above and below the Opalinus Clay indicated low hydraulic conductivities. Hydraulic conductivity obtained from the packer tests indicated typical values in the range between $1\text{E-}11$ and $1\text{E-}14$ m/s in the clay-rich sequences (Fig. 3-35). Intervals with clay mineral contents above about 40 wt.% have consistently low hydraulic conductivities ($< 10^{-13}$ m/s). Intervals with minimum clay contents of 20 wt.% are characterised by a somewhat larger scatter, while average hydraulic conductivities remain below 10^{-11} m/s, even if the test interval includes small-scale fault zones. This indicates a reduced (in comparison to the clay-rich intervals) but relevant self-sealing potential.

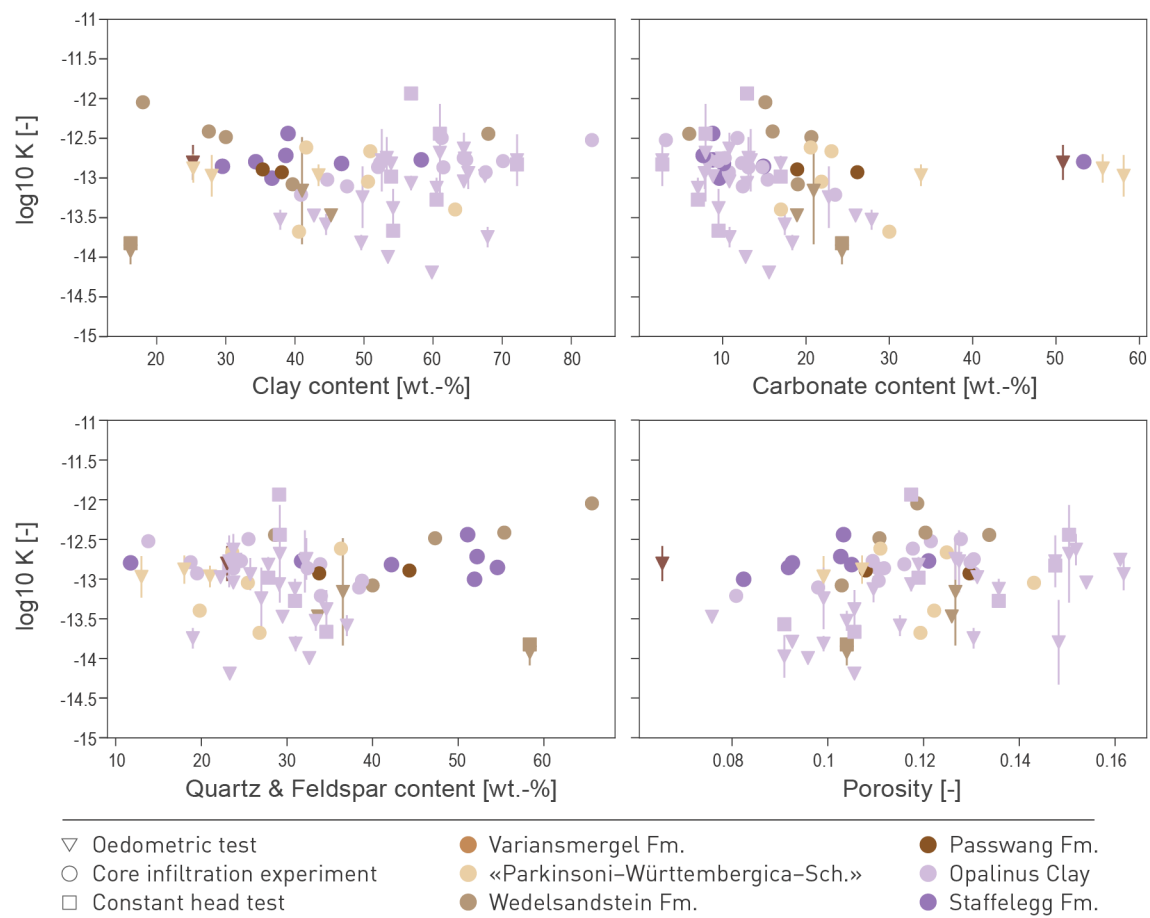


Fig. 3-34: Matrix hydraulic conductivity perpendicular to bedding for the confining geological units (Dogger and Lias) and the Opalinus Clay (From Nagra 2024b).

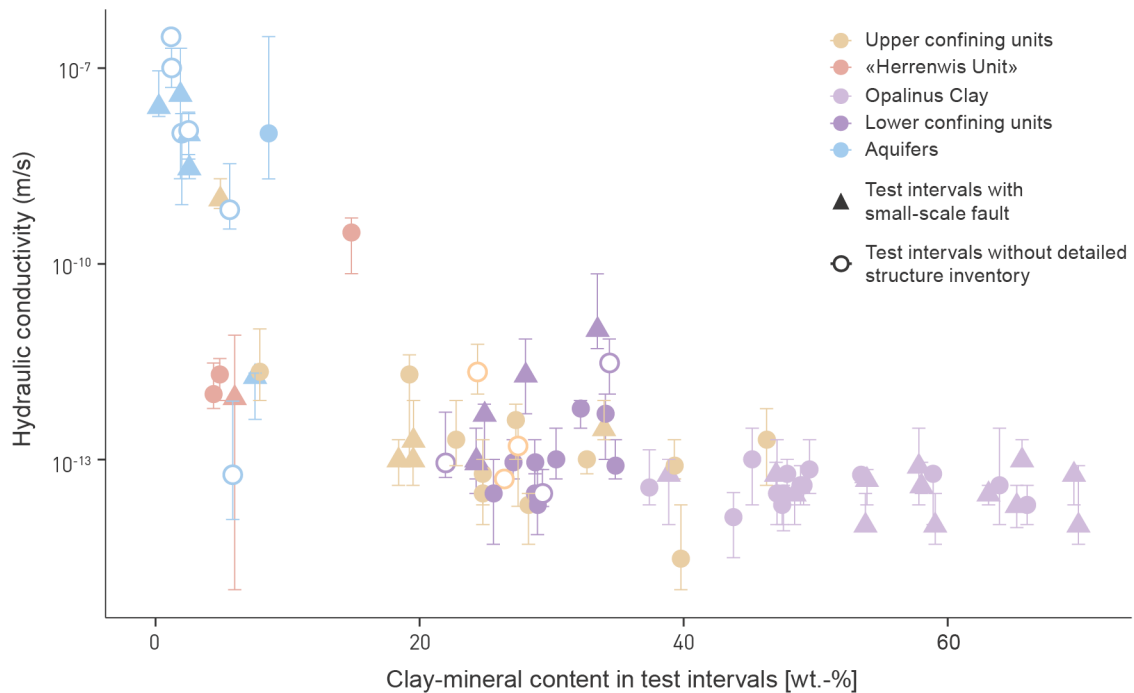


Fig. 3-35: Average hydraulic conductivity of the in-situ hydraulic packer tests as a function of the average clay content in the clay-poorest 5-m-layer in test intervals (From Nagra 2024b).

3.3.2 Gas-related characteristics of the clay-rich confining geological units

EPFL (Ferrari et al. 2012) and UPC (Romero & Gómez 2013) performed mercury intrusion porosimetry (MIP) on several core samples of the clay-rich sequences (so-called «Brauner Dogger» – BD) recovered from the Schlattingen borehole. The normalised pore-size distributions (PSD) from the MIP measurements of the different samples are shown in Fig. 3-36. Generally, the modes of the pore-size distributions of the BD core samples tend to be somewhat greater than those of the Opalinus Clay (Fig. 3-9, Fig. 3-10). For the calcareous zones of the upper confining geological units, the PSD curves are even smaller than those in the clay-rich sequences.

Water-retention curves (WRC) were measured on several core samples from the Schlattingen borehole (Ferrari et al. 2012, Romero & Gómez 2013). The water-retention data of the «Brauner Dogger» along the drying and wetting paths are plotted in Fig. 3-36. However, the fitted WRCs indicate a relatively high capillary strength parameter compared to the corresponding data from the Opalinus Clay. Similar to the Opalinus Clay, some hysteresis is indicated particularly for the WRCs based on the progressive method (see Ferrari et al. 2012). The WRC curves are representative of the unfractured rock matrix and do not take into account the expected decrease in capillary pressure in fractures.

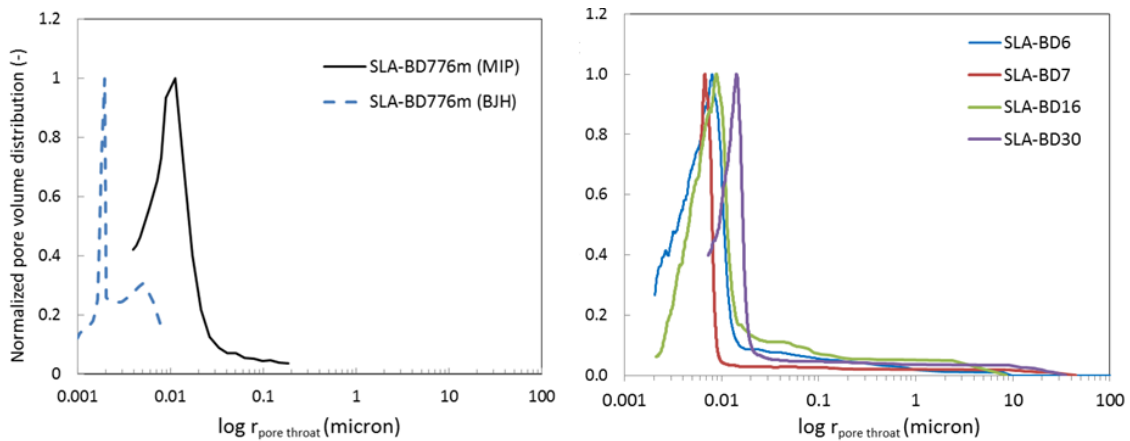


Fig. 3-36: Equivalent pore-size distributions (normalised) of drill-core samples from Schlattingen (sampling depth ranging from 766.7 to 807.4 m b.g.l.), determined by mercury-intrusion methods at EPFL (left) and UPC (right) and complemented with the BJH method

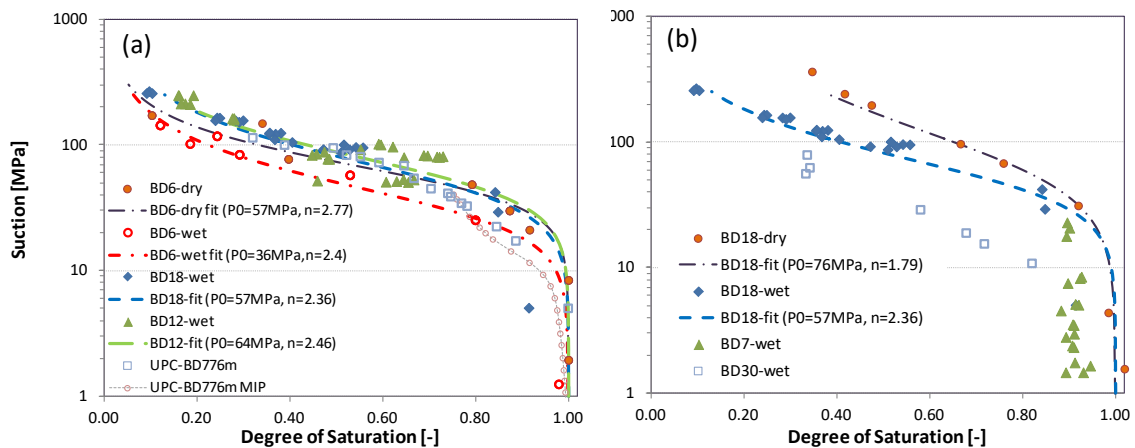


Fig. 3-37: Capillary-pressure measurements (water-retention curves) on a core samples from a clay-rich sequence of the upper confining geological units in the Schlattingen borehole

Tests were performed by means of stepwise desaturation and resaturation using a WP4c dew-point psychrometer and volumetric measurements (Ferrari et al. 2012, Romero & Gómez 2013): (a) using the Kerdane method; (b) using the progressive method for volume measurements.

Similar to the Opalinus Clay core samples from the Schlattingen borehole, two gas-injection tests were performed for a core sample from the upper confining units (sample OED 20 / 776.51 – 776.72 m b.g.l.; Parkinsoni-Württembergica Formation). The tests were conducted with flow direction perpendicular to bedding at isotropic stress levels of 15 and 19 MPa, respectively. The corresponding gas-injection pressures (14 and 18 MPa, respectively) remained below the confining stress. Fig. 3-38 presents the results of the tests in terms of gas pressures at the injection and outflow sides together with outflow volume and axial displacements.

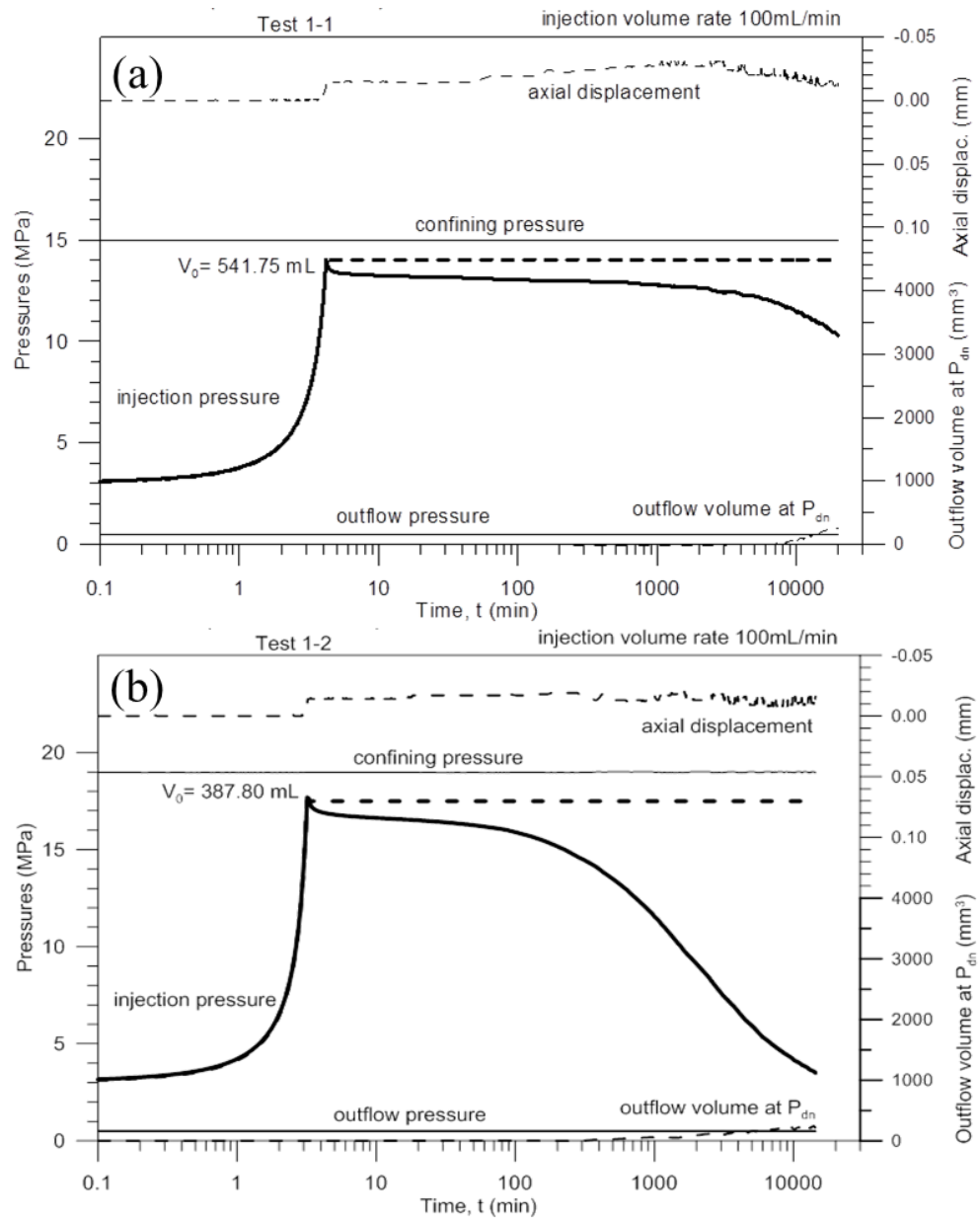


Fig. 3-38: Gas-injection experiments on core sample OED 20/«Brauner Dogger» (776.51 – 776.72 m) from the SLA-1 borehole

Measured time evolution of pressures at the injection and outflow sides together with outflow volume and axial displacements at confining pressures of (a) $p = 15$ MPa and (b) $p = 19$ MPa with isostatic stress conditions and flow orthogonal to bedding (from Romero & Gómez 2013).

The water-/air-permeability experiments on the BD sample show evidence for stress dependency of void ratio and water permeability. Despite its slightly higher intrinsic permeability, the samples from the clay-rich upper confining units underwent slightly lower air-dissipation rates during the recovery stage compared to the equivalent tests performed on the Opalinus Clay. As was the case for the Opalinus Clay samples, the BD sample displayed expansion at the early rapid air-injection stage in response to constitutive stress decrease, and dominant compression on air-pressure dissipation. Overall, the clay-rich upper confining geological units exhibit a less distinct stress coupling of hydro-mechanical properties than the Opalinus Clay.

3.3.3 Reference parameters for the clay-rich sequences of the confining geological units

The clay-rich sequences of the confining units exhibit similar hydrogeological characteristics as the Opalinus Clay. Beyond that, hydrogeological evidence suggests that brittle (tectonic) structures in the layers of limestones and sandy-calcareous marls can form discrete water-conducting features of limited fracture transmissivity, contributing to the overall porewater flow in the formation (“fracture flow”). The clustering of the observed brittle structures implies a slightly enhanced spatial variability of porewater flow in the hydraulic fracture network.

Representative hydraulic databases were compiled and the corresponding hydraulic reference parameters for the clay-rich sequences of the confining geological units were derived. Different sets of reference parameters were specified for the clay-rich marls and the sandy-calcareous sequences, respectively. Accordingly, two sets of gas-related reference parameters have been elaborated (Tab. 3-8). The parametric models used for the capillary-saturation relationship and the relative permeability of the clay-rich sequences are shown in Fig. 3-39 (reference values according to Tab. 3-8).

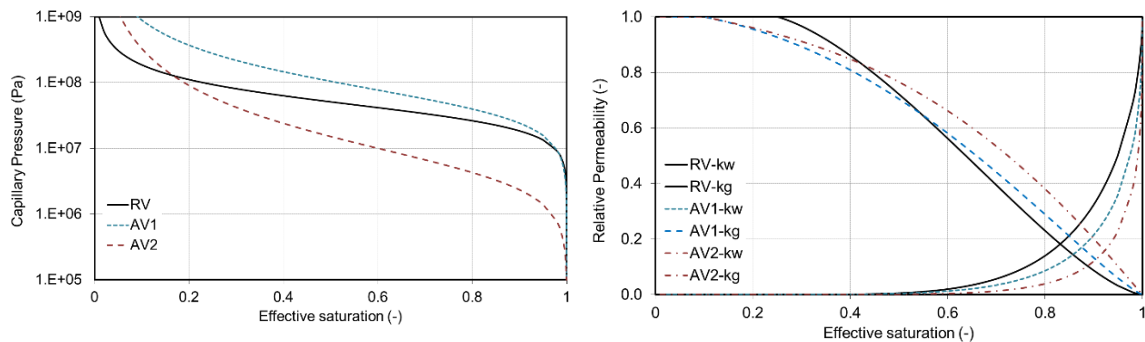


Fig. 3-39: Parametric models of capillary pressure and relative permeability k_r for water (w) and gas (g), representative of the clay-rich sequences of the confining geological units

RV = reference parameter values and AV1 and AV2 = alternative values.

Tab. 3-8: Reference values for the gas-related parameters of the clay-rich sequences of the confining geological units in Northern Switzerland

RV = reference value, AV = alternative value.

Parameter	RV	AV	Remarks
Undisturbed host rock			
Intrinsic permeability (clay-rich marls ⁽¹⁾ , sandy-calcareous marls ⁽²⁾) $k_{\perp}$ [m ²]	1×10^{-20} (1) 1×10^{-19} (2)	1×10^{-18} (1) 1×10^{-19} (2)	RV: corresponds to the reference value of hydraulic conductivity for clay-rich/sandy-calcareous marls. AV: representation as a homogeneous and anisotropic porous medium.
Anisotropy coefficient $k_{\parallel}/k_{\perp}$	1	10	RV: isotropic AV: same as Opalinus Clay
Capillary pressure-saturation relationship			Parametric model according to van Genuchten (Eq. 2-14).
Capillary strength P_o [MPa] (no distinction between clay-rich/sandy-calcareous marls)	36	50^{1*} 4.6^{2*}	RV: derived from WRCs (lowest wetting path), (Ferrari et al. 2012), accounting for fractures. AV1*: derived from WRCs by EPFL and UPC (representative of matrix). AV2*: assumed value, derived from field tests in sandy facies of the Opalinus Clay (Marschall et al. 2005).
Shape parameter n (no distinction between clay-rich/sandy-calcareous marls)	2.4	1.8^{1*} 1.54^{2*}	RV: derived from WRCs. AV1*: lowest value from WRC fits. AV2*: assumed value, derived from field tests in sandy facies of the Opalinus Clay (Marschall et al. 2005).
Relative permeability-saturation relationship			Parametric model according to van Genuchten/Mualem (Eq. 2-14 & 2-15) using the shape parameter n from the P_c - S curve.
Residual water saturation S_{wr} [-]	0.25	0.1	RV: reduced from MIP data to account for fracture effect. AV: assuming that most porewater is mobile
Residual gas saturation S_{gr} [-]	0.00	0.00	RV: effective gas entry pressure of the rock is infinitesimal. AV: -
Total porosity [%]	10%	8%	RV: porosity measurements from Schlattigen cores (see Fig. 3-11). AV: corresponds to the lower value in BD at depth.

3.3.4 Basic geological characteristics of the calcareous marls and limestones

The Wildegg Formation, Staffelegg Formation and Klettgau Formation comprise calcareous marls and limestones with low permeability and low porosity of the intact rock matrix. In the potential Jura-Südfuss siting region (Stage 1 of the SGT, set aside at a later stage), the Effingen Member of the Wildegg formation was a host rock for an L/ILW repository. In Stage 3 of the SGT, the calcareous sequences are part of the confining geological units, contributing to the overall barrier function of the geosphere.

Brittle tectonic features (faults) represent potential water-conducting features in the calcareous marls and limestones. In such formations with very low matrix conductivity of the intact rock, the interconnected network of water-conducting features exhibits the main body for porewater flow, controlling the effective hydraulic conductivity of the rock. The lithostratigraphic and hydrogeological characterisation of the calcareous marls and limestones is reported in Nagra (2024b) (see also Fig. 3-2, Fig. 3-33, Fig. 3-34 and Fig. 3-35).

3.3.5 Gas-related characteristics of the calcareous marls and limestones

Gas transport in the calcareous marls and limestones is governed by sedimentological and structural features on scales ranging between kilometres and micrometres. Thus, geophysical logs (Fig. 3-33) indicate a distinct variability of clay content with large horizontal correlation lengths. On the microscale, clear evidence is found for a distinct internal variability of the facies (Keller et al. 2013b, see Appendix B in Senger et al. 2013). Structural analyses by Mazurek (2013), drawing on core data from the Gösgen, Oftringen and Küttigen boreholes in the former Jura-Südfuss siting region and outcrop mapping in the Jakobsberg and Schümel quarries reveal a comprehensive inventory of discrete water-conducting features. The regional field study by Madritsch & Hammer (2012) complements the structural database with particular emphasis on large-scale fault systems. Fig. 3-40 exhibits examples of property distributions in the Effingen Member of the Wildegg Formation on observation scales, ranging between hectometres and micrometres.

Keller et al. (2013b) (see Appendix B in Senger et al.) performed microstructural analyses on a core sample from the Effingen Member in the Schlattigen 1 borehole (sample ID ZHAW; 738.70 – 739.02 m). The microstructural characterisation was based on focused ion-beam nanotomography (FIB-nt) in combination with broad ion-beam imaging (BIB). Two subsamples were subjected to an FIB-nt analysis by acquiring a sequence of cross-sectional SEM images spaced evenly throughout a region of a bulk specimen, and reconstructing those two-dimensional images into a three-dimensional representation of the sampled volume. The spatial resolution of the reconstructed image was 20 nm (voxel size) and the investigated volume was 1,275 μm^3 (around $10 \times 10 \times 10 \mu\text{m}^3$). Fig. 3-41 displays the results of the microstructural analyses of subsample number 2 by decomposing the sample volume (backscatter image in Fig. 3-41a) in a fraction of non-clayey grains (Fig. 3-41b), a clay fraction (Fig. 3-41c) and a pore network (Fig. 3-41d). The clay fraction fills the space between the non-clayey grains. The pore network displays only those pores with a pore radius > 20 nm, whereas smaller pores cannot be resolved (voxel size of the FIB-nt analysis).

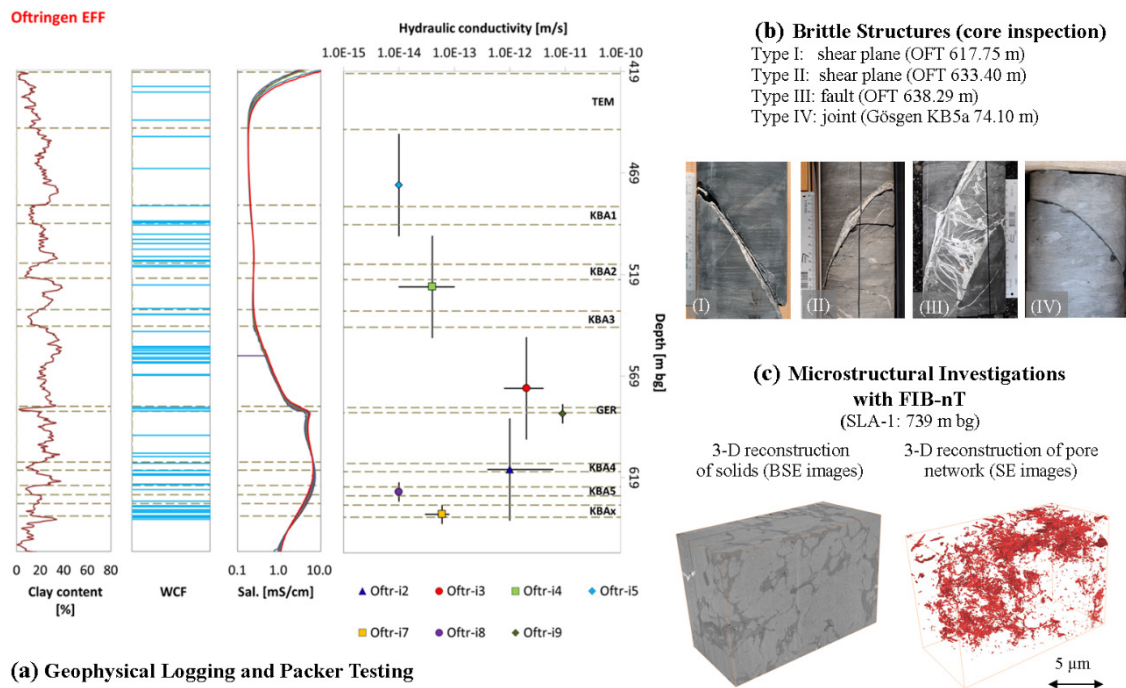


Fig. 3-40: Property distributions and relevant scales in the Effingen Member, representing the calcareous marls and limestones in the upper confining units

(a) Clay profiles, structural logs, fluid logging and packer testing in the Oftringen borehole; (b) brittle structures derived from core inspection; (c) microstructural investigations on core samples from the SLA-1 borehole.

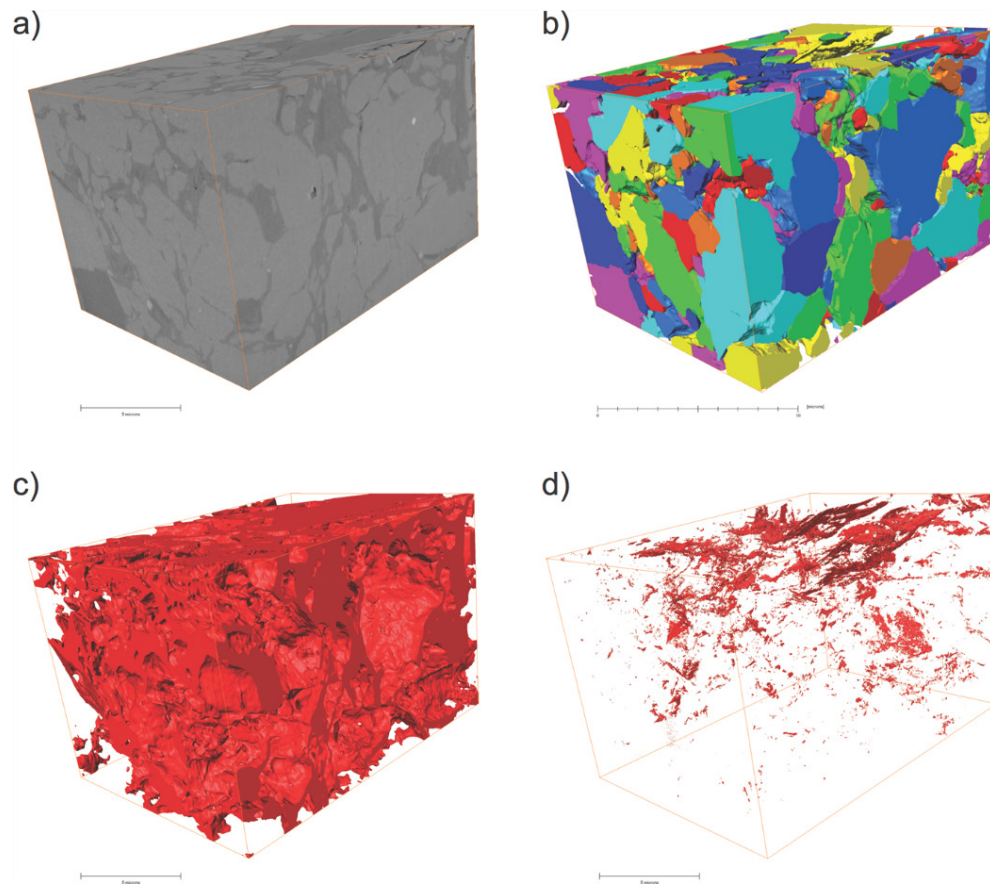


Fig. 3-41: Microstructural analysis of the rock matrix of the Effingen Member by FIB-nt

(a) 3D reconstruction of the analysed volume ($1,270 \mu\text{m}^3$); (b) 3D reconstruction of the framework of the non-clayey grains. Colours are label colours of individual grains; (c) 3D structure of the clay matrix; (d) 3D reconstruction of the pore space with pore radii $> 20 \text{ nm}$.

For the Effingen Member, mercury-intrusion porosimetry (MIP) was performed on a single core sample from the Schlattingen borehole (Ferrari et al. 2012) and on several samples from Oftringen and from Gösgen (Mazurek et al. 2012). The normalised pore-size distributions (PSD) from the MIP measurements of the different samples are shown in Fig. 3-42.

Water-retention curves (WRC) were measured on a single core sample from the Schlattingen borehole (Ferrari et al. 2012). The water-retention data of the Effingen Member along the drying and wetting paths are plotted in Fig. 3-43, indicating significant hysteresis. The fitted WRCs indicate a relatively high capillary-strength parameter, representative of the predominant clay-silt matrix and not the potentially fracture-dominated calcareous marls.

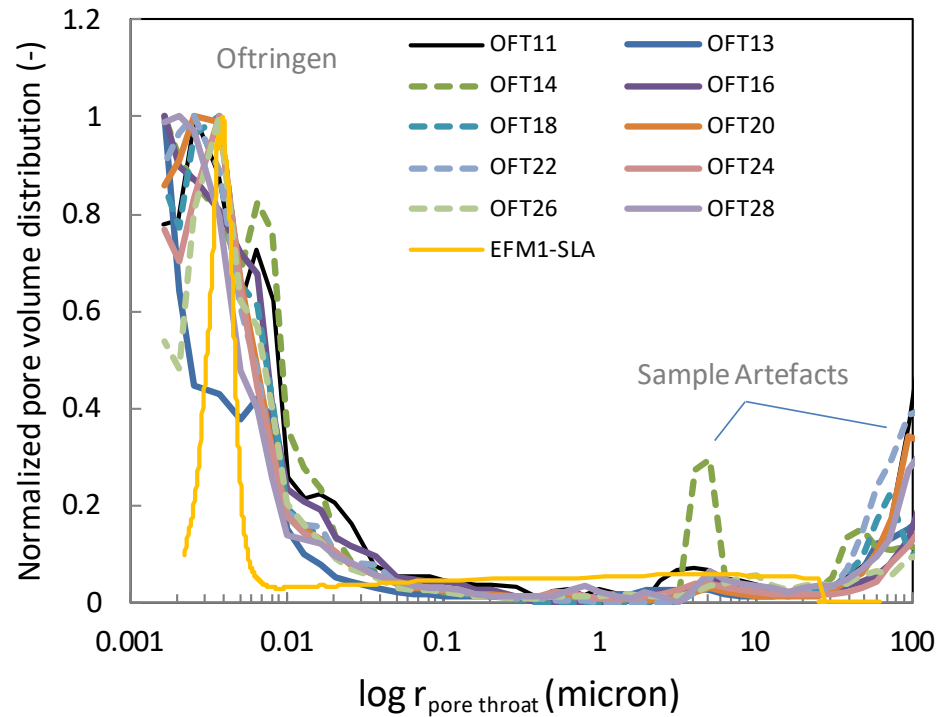


Fig. 3-42: Normalised pore-size distributions of core samples from the Effingen Member determined by mercury intrusion methods

The drill cores were recovered from the Oftringen borehole (Mazurek et al. 2012) and from the Schlattingen borehole (Ferrari et al. 2012).

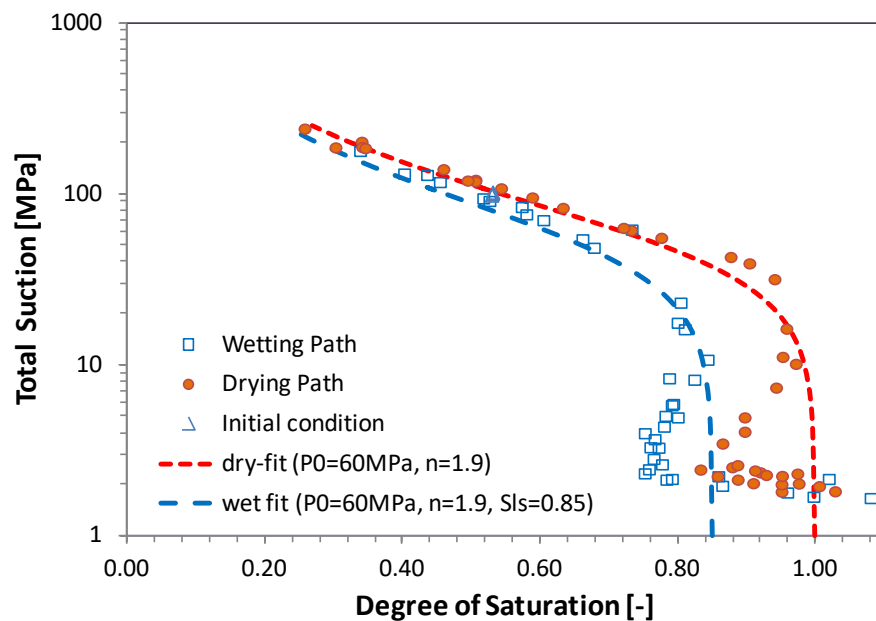


Fig. 3-43: Capillary pressure measurements (water-retention curves)

Workflow: stepwise desaturation and resaturation using a WP4c dew-point psychrometer, volumetric measurements using the same progressive method (Ferrari et al. 2012).

3.3.6 Reference parameters for calcareous marls and limestones

Porewater flow in the calcareous marls and limestones is controlled by the spatial variability of hydraulic conductivity governed by (i) the variability of porosity and clay content in the sedimentary structures (relevant for matrix flow); and (ii) the occurrence of brittle tectonic features (relevant for fracture flow). A previous site investigation programme in the context of Stage 3 of the SGT was dedicated to the hydraulic characterisation of the Effingen Member, i.e., a potential host rock formation in the former Jura-Südfuss siting region. The investigations included a comprehensive gas-related database (Senger et al. 2013), which is considered to adequately represent the two-phase flow characteristics of the calcareous sequences in the NL siting region. In the Jura-Südfuss siting region, high-interval transmissivities in packer tests were linked exclusively to test intervals in the argillaceous limestones (Gerstenhübel Beds (GER) and limestone bed sequences (KBA)), suggesting that fracture flow dominates in those lithologies. In the calcareous marl sequences (KMA), the interval transmissivities are generally low, which is regarded as a strong indication for matrix flow.

Different sets of reference parameters were specified for the KMA, KBA and GER, based on the derived average hydraulic conductivities of the different sequences, which are summarised in Tab. 3-9. In terms of two-phase flow parameters, the WRC data are representative of the low-permeability KMA, whereas the capillary-strength parameter is scaled to lower values for the higher permeable KBA and GER (Fig. 3-44).

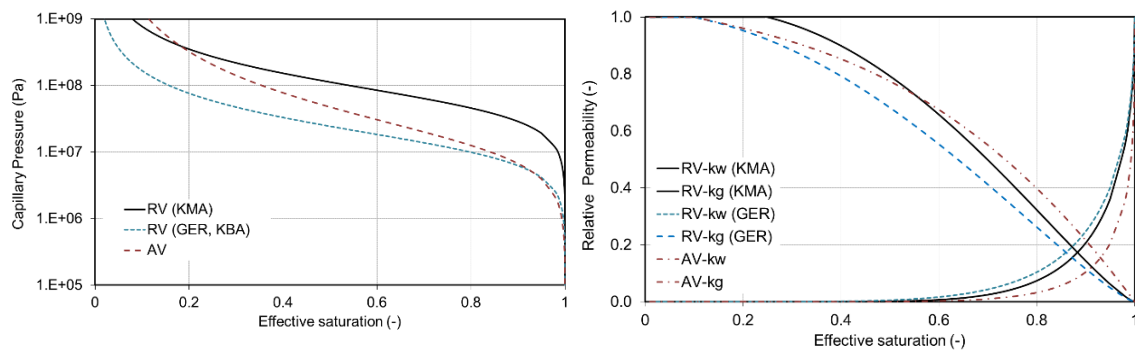


Fig. 3-44: Parametric models of capillary pressure and relative permeability k_r for water (w) and gas (g), representative of the Effingen Member

RV = reference parameter values, AV = alternative values.

Tab. 3-9: Reference values for the gas-related parameters of the Effingen Member in the former Jura-Südfuss siting region in Northern Switzerland

RV = reference value, AV = alternative value.

Parameter	RV	AV	Remarks
Undisturbed host rock			
Intrinsic permeability (KMA ⁽¹⁾ , KBA ⁽²⁾ , GER ⁽³⁾) k _⊥ [m ²]	1×10 ⁻²⁰ (1) 1×10 ⁻¹⁹ (2) 1×10 ⁻¹⁹ (3)	1×10 ⁻¹⁹ (1) 1×10 ⁻¹⁸ (2) 1×10 ⁻¹⁸ (3)	RV: corresponds to the reference value for hydraulic conductivity of calcareous marl sequences (KMA), limestone bed sequences (KBA) and Gerstenhübel Beds (GER). AV: corresponds to the value for hydraulic conductivity for the background fractures.
Anisotropy coefficient k _∥ /k _⊥	1	10	RV: no anisotropy assumed. AV: effect of intermittent sand beds expressed as anisotropic permeability.
Capillary pressure-saturation relationship			Parametric model according to van Genuchten (Eq. 2-14).
Capillary strength 1/α [MPa] (no distinction between KBA ⁽¹⁾ , KMA ⁽²⁾ , GER ⁽³⁾)	60 ⁽¹⁾ 13 ^(2,3)	13	RV: derived from WRC measurements (EPFL). AV: mean value for 2D model used in Papafotiou et al. (2011); values for 2D heterogeneous field, scaled using Leverett Function.
Shape parameter <i>n</i> (no distinction between KBA, KMA and GER)	1.9	1.5	RV: derived from WRC measurements (EPFL). AV: value used in Papafotiou et al. (2011).
Relative permeability-saturation relationship			Parametric model according to van Genuchten/Mualem (Eq. 2-15) using the shape parameter <i>n</i> from the Pc-S curve.
Residual water saturation S _{wr} [-]	0.25	0.1	RV: lower values than expected based on MIP due to fracturing. AV: assuming that nearly all porewater is mobile.
Residual gas saturation S _{gr} [-]	0.00	-	RV: assuming all porewater is mobile.
Water loss porosity [%]	8% ⁽¹⁾ 5% ⁽²⁾⁽³⁾	5%	RV: based on porosity measurements by Mazurek (2011). AV: corresponds to the lower value in matrix.

3.4 Additional, externally obtained evidence

3.4.1 Additional evidence for Opalinus Clay and similar rocks from the EURATOM 7th Framework Project – FORGE (2010 – 2013)

The FORGE project (2010 – 2013) was a European project with links to international radioactive waste management organisations, regulators and academia. It was specifically designed to tackle the key research issues associated with the generation and movement of repository gases. Of particular importance were the long-term performance of bentonite buffers, plastic clays, indurated mudrocks and crystalline formations. Comprehensive experimental data were acquired to reduce uncertainty relating to the quantitative treatment of gas within the framework of performance assessment. FORGE addressed these issues through a series of laboratory and field-scale experiments, including the development of new methods for upscaling, allowing the optimisation of concepts through detailed scenario analysis (Norris et al. 2013). Further details on the FORGE project and its outcomes can be accessed at <http://www.FORGEproject.org>.

Work packages 4 and 5 of the FORGE project were dedicated to the investigation of gas transport processes in the disturbed and intact host rock, respectively. New experimental databases were derived from gas-related laboratory and in-situ experiments in the Opalinus Clay, Calovo-Oxfordian, and Boom Clay. The experiments were modelled using numerical codes with advanced THM features. A brief summary of the experimental achievements is given below.

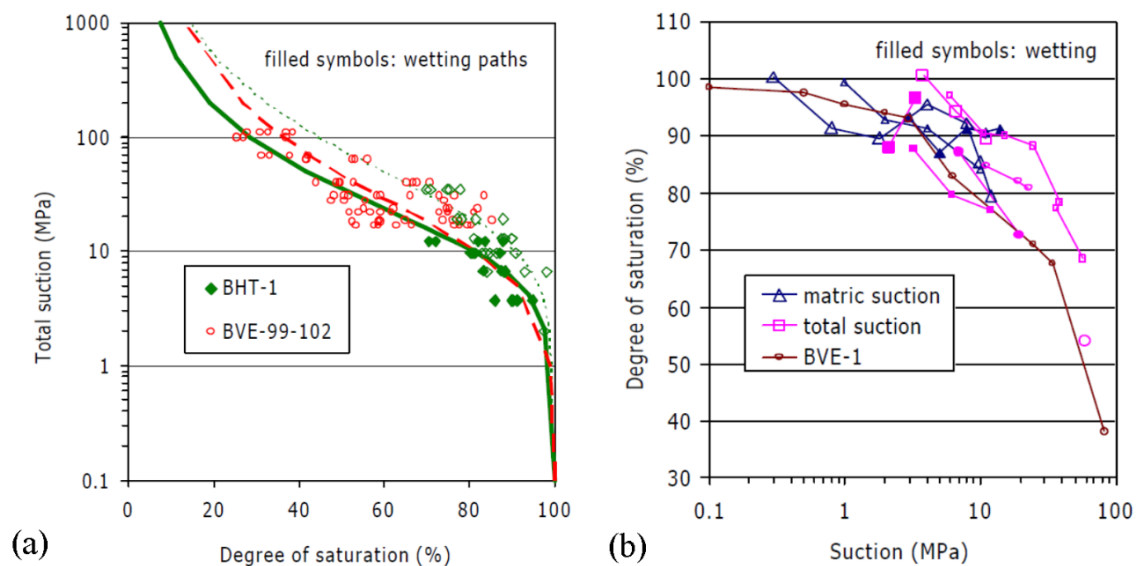


Fig. 3-45: Water-retention measurements on core samples from Mont Terri

(From Villar & Romero 2012).

(a) WRC along wetting/drying paths obtained under free volume conditions; van Genuchten curves are fitted to the different datasets. (b) WRC obtained under confinement (oedometric cell, 8 MPa vertical stress for samples from BHG-D1 and BHT-D1 boreholes; constant volume conditions for BVE-1 samples). The samples from the BVE-1 borehole were subjected to drying paths applying total suction (for suctions above 3 MPa) or matric suction (for suctions below 3 MPa) while keeping their volume constant in the oedometer.

Villar & Romero (2012) derived water-retention curves of Opalinus Clay samples from Mont Terri (BHT-1 and BHG-D1 boreholes) and compared their results with previous studies (Mont Terri: BVE-1, BE-99 – 102 boreholes). The WRCs were determined under different conditions: total and matric suction, free volume or confined volume, wetting and drying paths. The data were matched with a van Genuchten parameter model. Results of the study are presented in Fig. 3-45. Overall, a good agreement is seen with the water-retention curves, which were determined by EPFL and UPC (see Fig. 3-11).

Villar et al. (2013) designed an experimental setup to measure gas-permeability and gas-breakthrough pressures in highly confined Opalinus Clay samples. The maximum gas-injection pressures and confining pressures were 20 MPa and 30 MPa, respectively. Gas outflow was measured with a resolution of about 0.04 cm³/min (STP). A series of water-/gas-permeability tests was performed on rock samples from Mont Terri (BDR-1 borehole) perpendicularly to the bedding plane. The authors derived an intrinsic permeability of 1E-20 m² from water-injection tests. Furthermore, the breakthrough pressure of samples with a saturation degree of 84 ± 15% was above 18 MPa. The air-entry value calculated from the mercury-intrusion porosimetry tests was 28 MPa. The reported effective gas permeabilities (i.e., intrinsic permeability times relative gas permeability) ranged from 1E-20 to 1E-24 m². These results are broadly consistent with the results reported in Section 3.2.2. Nevertheless, it should be noted that the authors point out the pilot character of the experiments, particularly raising questions on mass-flow resolution of the gas flowmeter.

3.4.2 Additional evidence for Callovo-Oxfordian (COx) from the EURATOM 7th Framework Project and EURAD WP GAS

The microstructure of COx claystone, crucial for understanding gas transfer, consists mainly of a clay matrix with interparticle and interaggregate pores, and interlayer porosity in swelling clays. The pore network ranges from 1 nm to a few hundred nanometres (Sammartino et al. 2003, Yven et al. 2007). At the macroscopic scale, COx claystone exhibits anisotropy relative to the bedding plane. Various experimental techniques, such as nuclear magnetic resonance (NMR), mercury-intrusion porosimetry (MIP), gas/water adsorption, X-ray microtomography (μ-CT), focused ion-beam-scanning electron microscopy (FIB-SEM) and transmission-electron microscopy (TEM) were used to study porosity at different scales (Song et al. 2015).

Gas-entry pressure measurements on COx samples, under varied conditions, revealed two groups of values: 0.3 – 3 MPa for damaged material and ≥ 5 MPa for sound COx claystone (Robinet 2008, Song et al. 2015). Considering microstructure and porous network connectivity, actual breakthrough pressure could be higher, i.e., estimated to be between 6 and 10 MPa. Rigorous sample handling is crucial due to gas sensitivity to microcracks, requiring a careful protocol to avoid underestimating gas-entry pressure. Water-retention curves for COx were obtained by monitoring sample mass in controlled humidity atmospheres, with hysteresis effects observed (Fig. 3-46).

Effective gas-permeability measurements in COx (Zhang et al. 2002, Yang 2008, Boulin 2008, Gérard 2011, Didier 2012) showed dispersion, primarily influenced by local damages. Calibration of permeability curves focused on samples with limited cracking effects (Fig. 3-47). Klinkenberg correction, accounting for gas slippage along pore walls, was applied to gas-permeability measurements, which are especially significant at low pressures. Klinkenberg coefficient measurements indicated reduced correction with increasing water saturation (Boulin et al. 2008, Didier 2012).

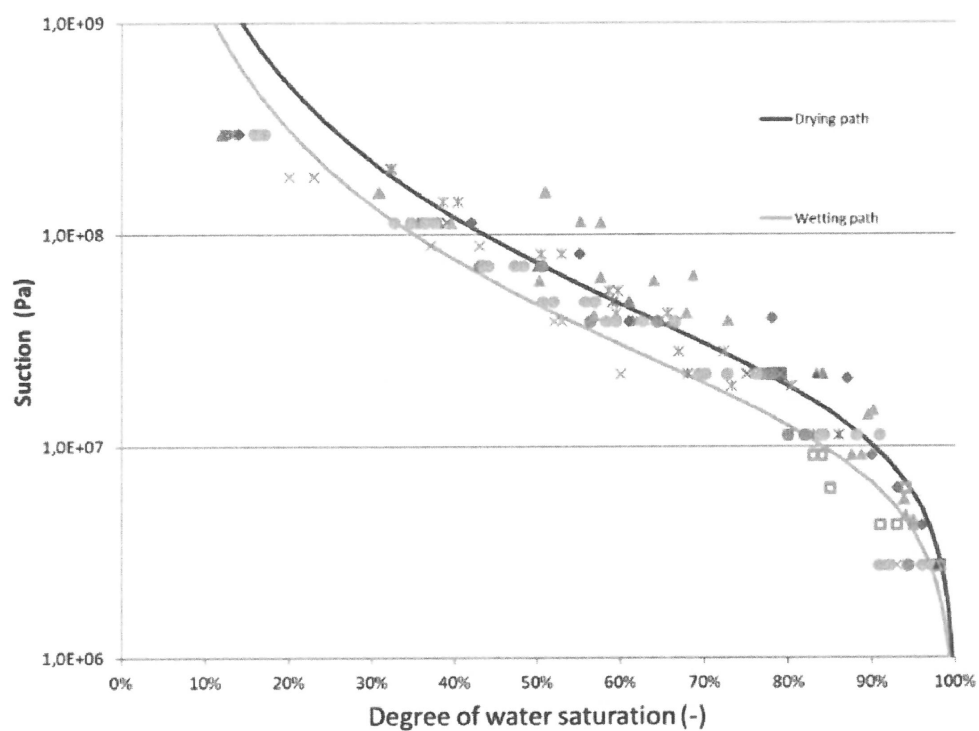


Fig. 3-46: Relation between water saturation and suction

Measurements obtained on several samples and fitted using a van Genuchten model on a drying path and wetting path for COx claystone (Armand et al. 2017).

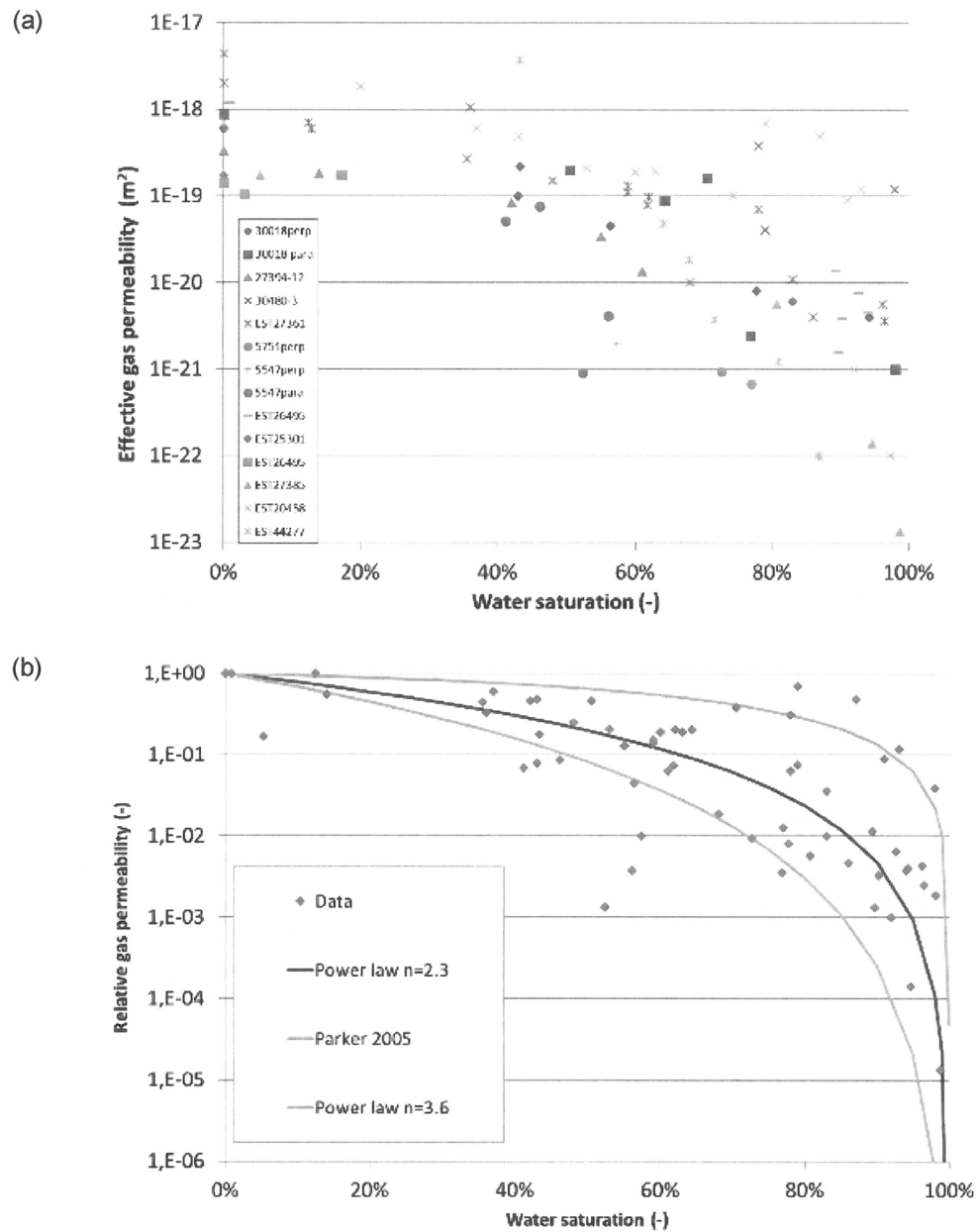


Fig. 3-47: Effective gas permeability as a function of water saturation

(a) Compilation of the dataset, (b) relative gas permeability fitting with power law and Parker approach.

Long-term water-/gas-injection tests were performed by the British Geological Survey on two rock samples (COx-1 and -2) from the Callovo-Oxfordian, the proposed host rock for the French repository (Harrington et al. 2012, Harrington 2013). A porewater backpressure of 4.5 MPa was continuously imposed at the top of the sample through the central filter, and an isotropic confining stress of 12.5 MPa was maintained during the entire experiment. The core specimen had an initial diameter of 54.4 mm and a height of 53.9 mm. The orientation of the sample was perpendicular to the bedding. More details about the experiment conditions can be found in Harrington et al. (2012). Hydraulic testing of sample COx-1 revealed a specific storage of $\sim 6\text{E-}6 \text{ m}^{-1}$ and axial/radial permeabilities of $\sim 2\text{E-}21 \text{ m}^2$ and $\sim 5\text{E-}21 \text{ m}^2$, respectively. Helium injection occurred

through the base of the sample by slowly increasing gas pressure in a series of steps (from 6.5 to 12 MPa) and then decreasing stages (from 12 to 7 MPa), while outflow evolution was measured at the top. Fig. 3-28 displays the slow, stepwise increase of gas-pressure gradient across sample COx-1 from 6.5 to 12.0 MPa over a 600-day period. A first small emergent flux during the early stages of testing was observed before a spontaneous increase of discharge rate after 170 days, which was interpreted as evidence of major breakthrough. The breakthrough was accompanied by a spontaneous increase in discharge rate, ultimately leading to a quasi-steady state flow rate.

Analysis of flux and pressure data indicates dynamic flow behaviour and time-dependent propagation of gas pathways across the specimen, made apparent by spontaneous changes in flux and guard-ring pressure (Fig. 3-48). Based on these observations, the excess gas-breakthrough pressure for the COx-1 sample was estimated to be ~ 2 MPa. In stark contrast, test COx-2 exhibits a gas-entry pressure in excess of 6 MPa, which may suggest a marked variability of gas-entry pressures in the Callovo-Oxfordian. Nevertheless, both tests reveal gas-entry pressures of the rock that are significantly below the confining stress of 12.5 MPa.

The test results of the laboratory experiments were modelled with an anisotropic hydro-mechanical model to take into account couplings between the pathways aperture, permeability and air-entry pressure and to explain the development of gas-localised pathways (Harrington 2013). Following the idea of the “embedded fracture model” of Olivella & Alonso (2008), in this model, permeability and air-entry pressure evolve with strain in order to give an appropriate representation of single fractures embedded in a continuous finite element matrix. According to Harrington (2013) the use of the “embedded fracture model” allows a more convincing simulation of the gas-breakthrough phase with high gas fluxes and the pressure recovery phase than could be achieved by classical two-phase flow codes. However, the definition of the pre-existing fracture geometry is based on experimental evidence and remains arbitrary. Modelling with other geometry of the pre-existing fracture has shown the ability of the model to reproduce localised pathways, but this requires adapting the set of parameters used (Harrington 2013).

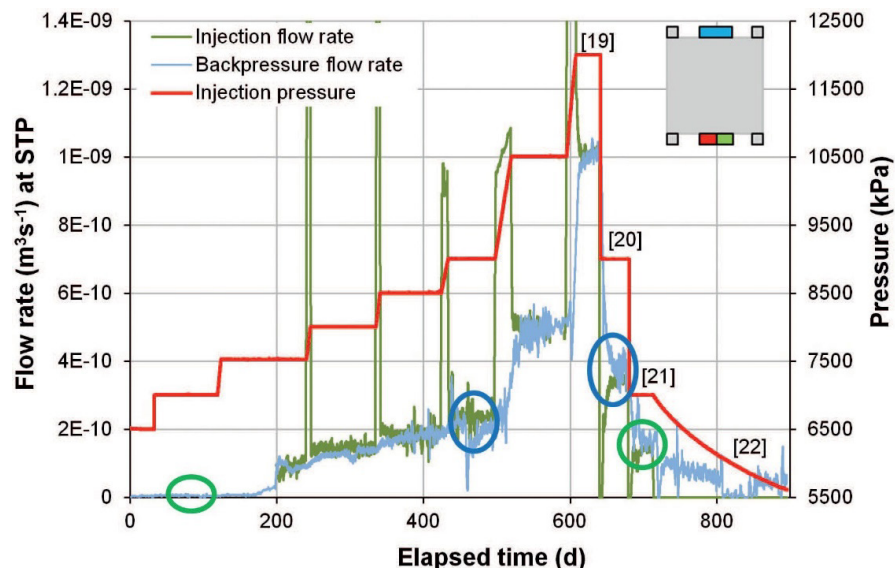


Fig. 3-48: Long-term gas-injection test on the rock samples from the Cox
(From Harrington et al. 2012).

Gas-flow rates at the injection and backpressure filters during the gas-injection test on COx-1. The large spikes in injection flux relate to the compression of the gas phase during constant flow-rate tests. The blue and green circles highlight hysteresis in the flow response.

3.4.3 Additional evidence for Boom Clay from the EURATOM 7th Framework Project and EURAD SOTA WP GAS

The Boom Clay pore network characteristics were studied through mercury-intrusion porosimetry (MIP) and nitrogen-adsorption tests (Gonzalez-Blanco 2017, Gonzalez-Blanco & Romero 2022). The MIP results revealed a dominant pore size at the intra-aggregate scale, around 70 nm, indicative of a matrix-type microstructure. The BJH method showed a smaller peak around 3 nm (Fig. 3-49).

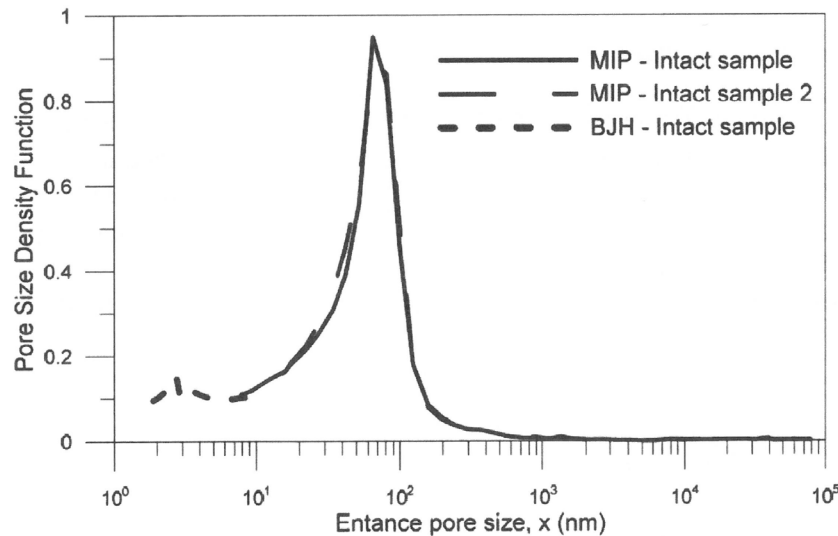


Fig. 3-49: Pore-size density function of intact Boom Clay samples
(From Gonzalez-Blanco 2017).

Water-retention curves were extensively investigated, and the Boom Clay water-retention curve was estimated using a dew-point psychrometer, showing consistency with the results from other laboratories. The curve, incorporating MIP data and psychrometer measurements, was fitted with van Genuchten's equation, with an air entry value of approximately 4.8 MPa (Fig. 3-50).

The intrinsic permeability of Boom Clay was determined through laboratory water and gas permeameter experiments. Water-intrinsic permeability consistently displayed lower values than air-intrinsic permeability, suggesting preferential pathways for air flow. The orientation of bedding planes influenced water-intrinsic permeability, emphasising the role of material deformation along injection and dissipation stages. The intrinsic permeability of Boom Clay and its retention curve depend on strains due to changes in pathway aperture. More recent analysis of water permeability (Gonzalez-Blanco & Romero 2022, Gonzalez-Blanco et al. 2024) estimated at in-situ stress level and after the drained loading to 6 MPa indicated a distinct increase with increasing void ratio (Fig. 3-51). It also showed higher water permeability with flow parallel to bedding planes, indicating a marked anisotropic feature.

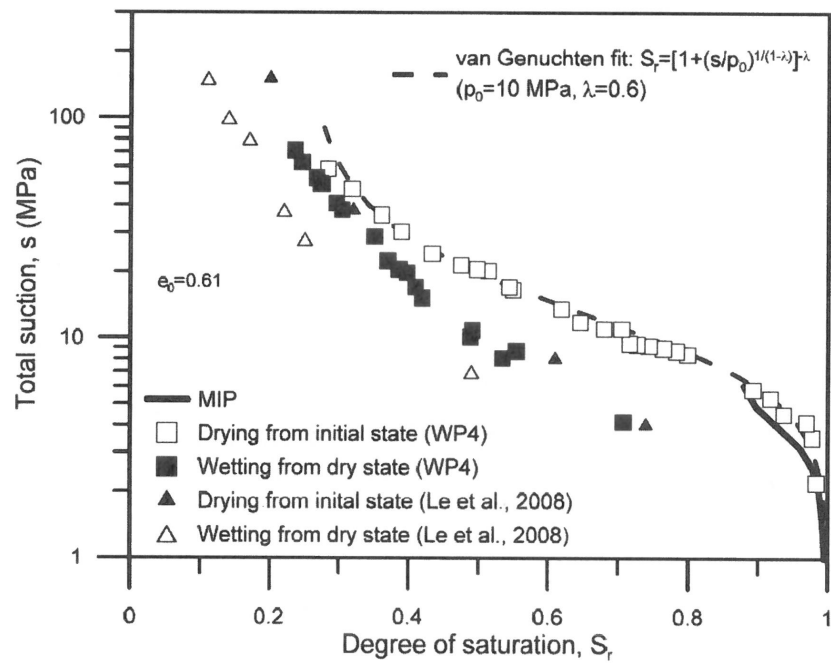


Fig. 3-50: Water-retention curve of the Boom Clay
(From Gonzalez-Blanco 2017).

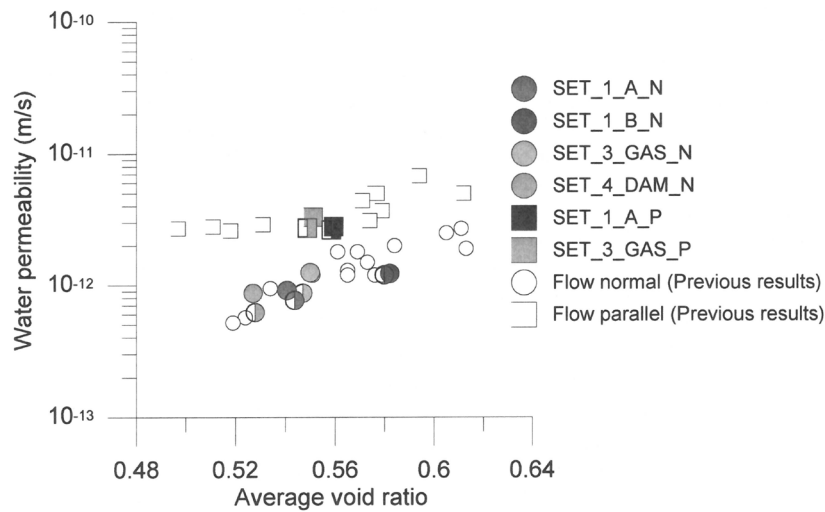


Fig. 3-51: Boom Clay – water-permeability results as a function of the void ratio

Relative permeability relationships for liquid and gaseous phases were made dependent on the degree of saturation using the van Genuchten model for liquid-relative permeability (Fig. 3-52). The gas-relative permeability of the Boom Clay can be expressed as a generalised power law (Delahaye & Alonso 2002). Gas flow in Boom Clay, influenced by visco-capillary forces, leads to an increase in pore space, affecting intrinsic permeability and capillary pressure-saturation relationships. In contrast to conventional two-phase flow, the transport properties of the solid phase become variable, depending on the state of deformation of the rock.

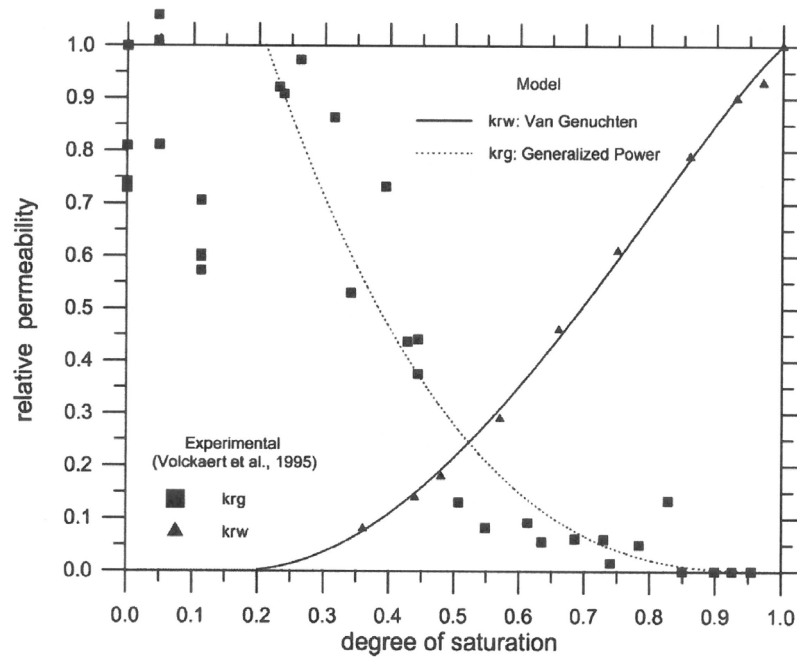


Fig. 3-52: Experimental data for relative permeability in Boom Clay (Volckaert et al. 1995) together with model fitting (Delahaye & Alonso 2002)

k_{rw} : relative permeability of water / liquid phase, k_{rg} : relative permeability of gas.

Gonzalez-Blanco & Romero (2022) and Gonzalez-Blanco et al. (2024) extended the experimental investigation with a multi-scale perspective on the response to gas transport of initially saturated Boom Clay (Belgium). Gas-injection tests have been performed under oedometric conditions at different controlled-volume rates, constant total vertical stress and different sample orientations (flow orthogonal or parallel to bedding planes). The results confirm soil expansion and consequent degradation during injection. This has a significant impact on the aperture of localised gas pathways (fissures) and increases intrinsic permeability during the gas-pressure dissipation stage. The analyses with complementary techniques (mercury-intrusion porosimetry, field-emission scanning-electron microscopy and X-ray microtomography) confirm the opening of fissures with different apertures and separations at the microstructural scale (Fig. 3-53). Large-aperture fissures develop along the weaker bedding planes (Fig. 3-54). These techniques allow the volume of fissures to be quantified, which does not significantly depend on gas flow direction, as also measured in the isotropic response of the gas-effective permeability which exhibits larger values than water permeability (Fig. 3-55). Sample SET 4 was subjected to a loading path that exceeded the yield stress, resulting in lower gas and water permeabilities that also indicated a decrease in porosity (Fig. 3-55).

The pore-size density curves obtained through mercury-intrusion porosimetry (MIP) for the intact state displayed a single-mode distribution with a predominant size of 70 nm and minimal volume at the macroscale (Fig. 3-56). However, following gas-injection tests in previous studies, a new family of larger pores, exceeding 2 μm , consistently emerged. These larger pores were associated with Boom Clay sample expansion and gas-pathway dilation during gas injection. Comparison of the PSD curves after resaturation (SET_1A) and after the second gas-injection stage (SET_1B and SET_3) shown in Fig. 3-56 indicate larger pore sizes. Post-resaturation, volumes at the macroscale were lower than after gas injection but slightly higher than intact samples, indicating incomplete material healing. Conversely, samples after the second gas injection exhibited the highest macroscale volume.

The differences between gas and water permeability are linked to the evolution of the microstructure in Boom Clay. To account for it, Gonzalez-Blanco et al. (2024) developed a simple model, using the volume of fissures and pores at the macroscale detected after the tests and related them to the permeability measured at the last stage of each test. A macrofissure fraction was defined to consider the changes in the microstructure as:

$$f = \frac{e_f + e_M}{e} \quad (3-12)$$

where e_f is the fissured void ratio (volume of fissures to the volume of solids (V_f/V_s)), e_M is the macro void ratio (volume of macropores to the volume of solids V_M/V_s) and e represents the void ratio at the end of the tests.

The permeability ratio was calculated for all the samples to correlate it with the macrofissure fraction f :

$$\frac{k}{k_{initial}} = [\alpha_i(f - f_0) + 1] \quad (3-31)$$

where f_0 represents the volume of the macropores at the intact state, which is independent of the bedding orientation and can be obtained with MIP data.

The proposed linear model relating the macrofissure ratio with the permeability ratio is shown in (Fig. 3-57), which shows (i) the formation of fissures during gas injection, leading to an increase in effective permeability; (ii) the subsequent closure of these fissures upon resaturation, resulting in the restoration of initial permeability, encompassing the unconnected macro-pores filled with occluded gas; and (iii) the enlargement of the macrofissure ratio upon successive injections, illustrating the simultaneous development of fissures and macropores, ultimately leading to the maximum gas permeability.

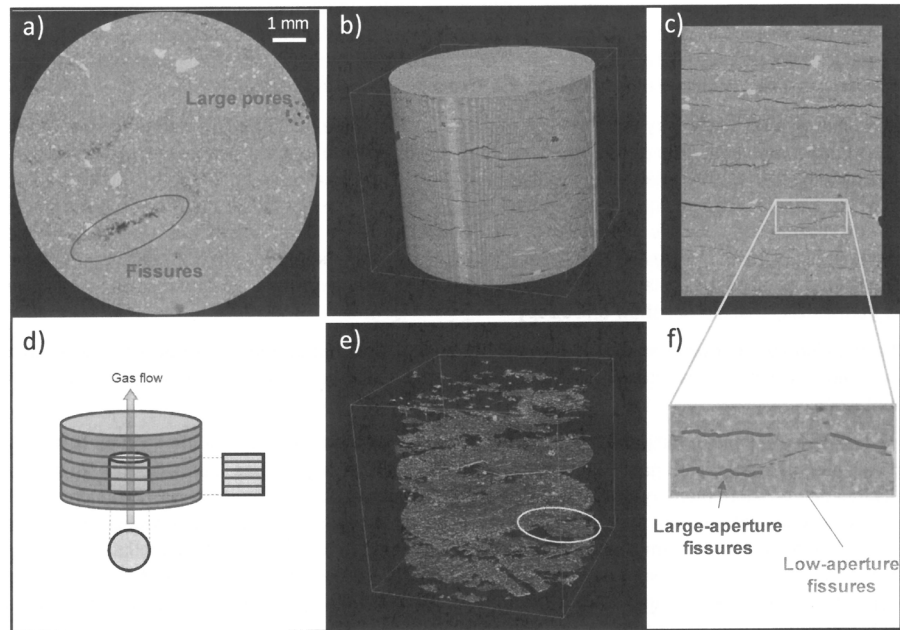


Fig. 3-53: μ -CT data of sample SET_1_B_N after second gas injection with improved resolution

a) Cross-section at mid-height; b) 3D volume reconstruction of μ -CT images; c) longitudinal section at the middle; d) subsampling scheme; e) porosity segmentation; and f) zoom showing a low-aperture fissure bridging large-aperture fissures.

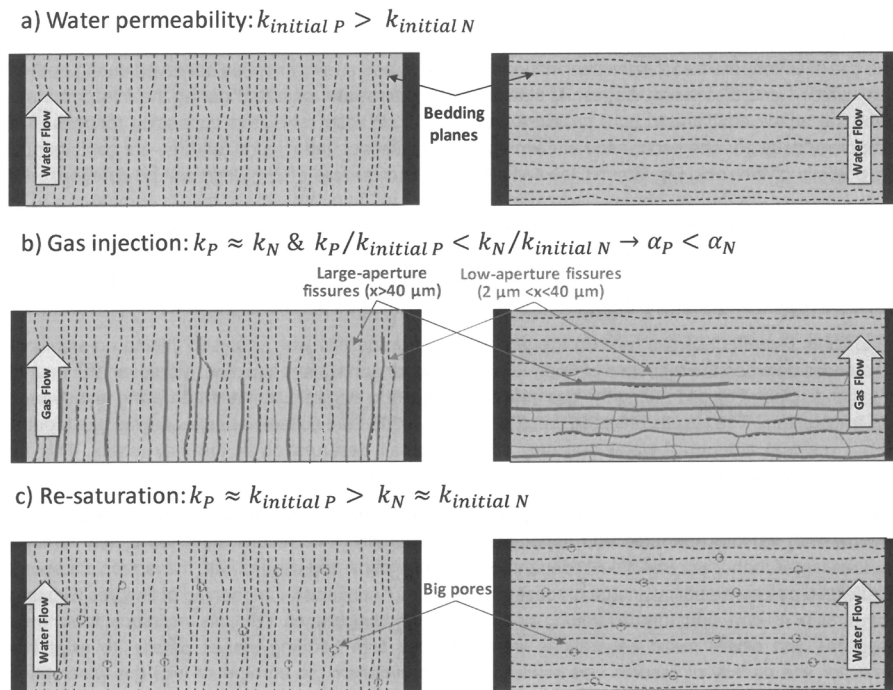


Fig. 3-54: Illustration of fluid transport during each process outlined by the model, highlighting key variables and parameters

Dashed lines denote bedding planes, continuous lines depict gas pathways, and circles symbolise pores containing entrapped gas.

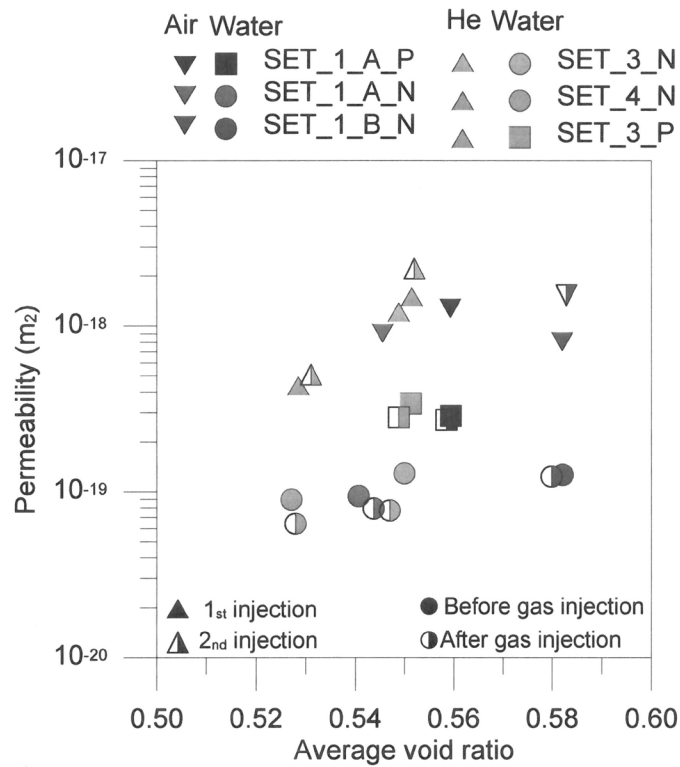


Fig. 3-55: Permeability of Boom Clay to water and gas against void ratio

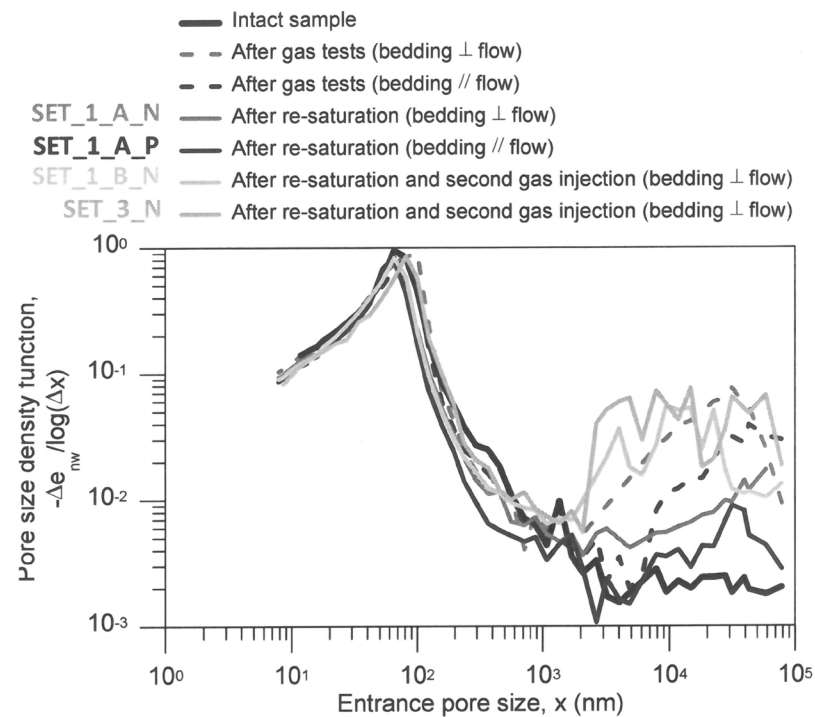


Fig. 3-56: Pore-size density curves from MIP on the intact sample, samples after gas-injection tests, samples after resaturation and samples after second gas injection

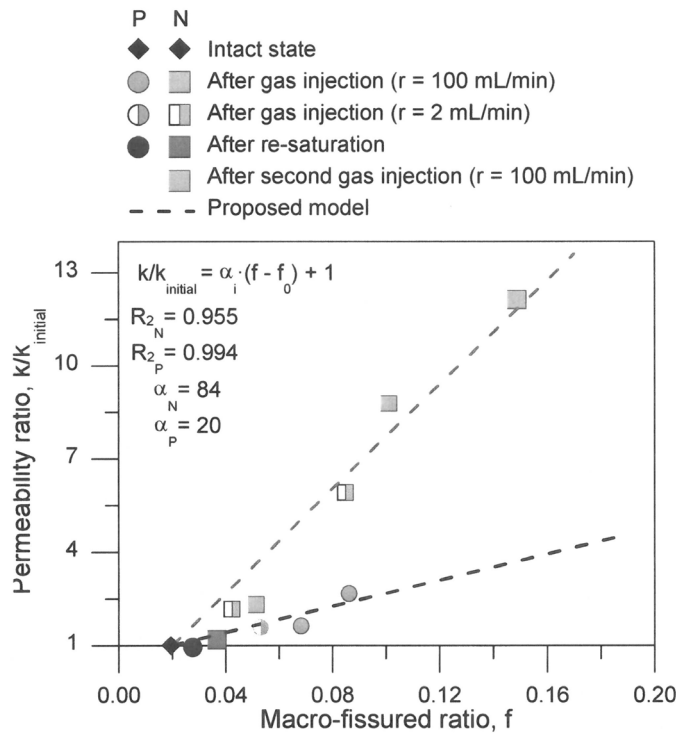


Fig. 3-57: Proposed linear model relating the macrofissured ratio with the permeability ratio for both bedding orientations

P: samples with bedding planes parallel to flow, N: samples with bedding planes normal to flow.

3.4.4 Complementary evidence from the oil and gas industry

Argillaceous formations such as shales and claystones represent the major constituents of sedimentary basins (e.g., Hildenbrand & Urai 2003). They form seals for hydrocarbon accumulations, aquitards and chemical barriers. A detailed knowledge about the sealing characteristics is of particular interest in petroleum science (e.g., Ingram et al. 1997; Ingram & Urai 1999). Further evidence for gas transport in clay-rich formations has been found in other areas such as natural gas storage and CO₂ sequestration. Benson et al. (2002) reviewed the safety results of underground storage in the United States as part of a comprehensive study considering CO₂ storage in deep geological formations. Another comprehensive literature study on gas storage and gas transport phenomena is given in Evans & West (2008).

Empirical investigations and phenomenological descriptions of gas flow through clay-rich seals were the subject of many geoscientific papers in the field of reservoir engineering (e.g., Clayton & Hay 1994, Zweigel et al. 2005). The extremely low intrinsic permeabilities of natural clay barriers (e.g., Neuzil 1994) and their high sealing capacity (Harrington & Horseman 1999) are controlled by the rock microstructure (a network of very small interconnected capillaries with pore neck radii down to the nm-range) and chemical interactions between minerals (e.g., smectite) and the permeating fluid.

The following paragraphs provide a brief survey of laboratory investigations on gas transport in low-permeability formations from other geoscientific disciplines.

Water-retention measurements/mercury porosimetry

In the oil and gas industry, MIP is the standard method for characterising the capillary strength of rocks. A multitude of papers have been published, presenting the results of MIP for a variety of shales, claystones and tight sandstone formations. In the subsequent paragraph, sample results from a comprehensive study of the Mesaverde Tight Gas Sandstones from Western U.S. Basins are discussed. The corresponding test protocols and the interpretation procedures are described in great detail in a scientific report by Byrnes et al. (2009).

Fig. 3-58a presents the capillary pressure curves for selected samples with permeabilities in the range of $2.5\text{E-}19\text{ m}^2$ – $2.24\text{E-}15\text{ m}^2$. Only the tightest samples exhibit a permeability comparable to the reference permeabilities of the candidate host rock formations of the Effingen Member and «Brauner Dogger», which were 1 to 2 orders higher than that of the Opalinus Clay. The capillary pressure curve of the tightest sample ($2.5\text{E-}19\text{ m}^2$) is comparable in shape and magnitude to the retention curves derived for the Opalinus Clay at Mont Terri (Fig. 3-12). Fig. 3-58b displays repeated drainage/imbibition curves for a low-permeability sandstone ($7\text{E-}19\text{ m}^2$) with a porosity of 5.9%. The capillary strength of the sample is in the order of several MPa. Furthermore, a distinct trapping of the invaded mercury is observed during the successive drainage/imbibition cycles, which can be seen as an indication of the poor connectivity of the pore network.

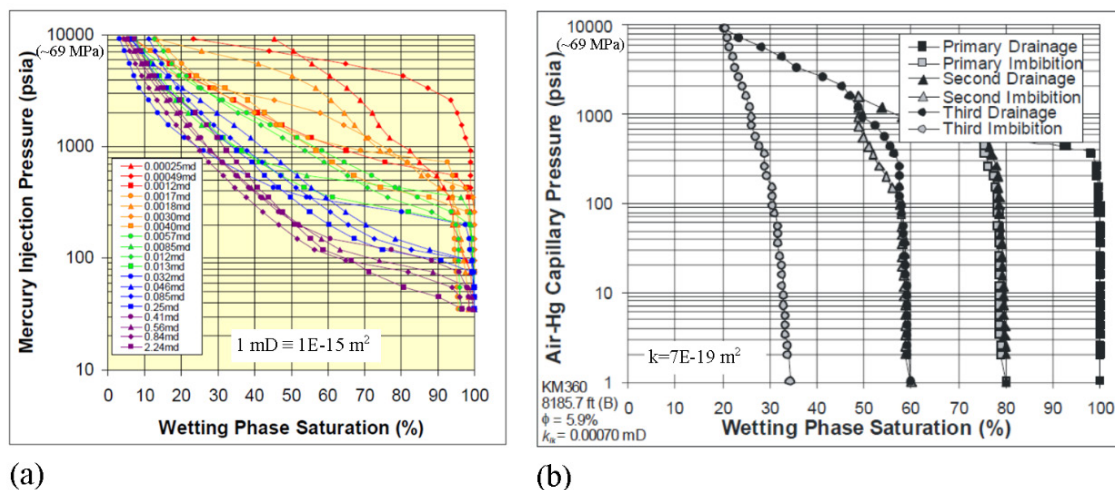


Fig. 3-58: Mesaverde Tight Gas Sandstones project

(After Byrnes et al. 2009).

(a) Air-mercury capillary pressure curves for selected samples ranging in permeability from 0.00025 mD to 2.24 mD (corresponding to $2.5\text{E-}19\text{ m}^2$ – $2.24\text{E-}15\text{ m}^2$). The curves exhibit increasing threshold entry pressure and increasing “irreducible” wetting-phase saturation with decreasing permeability; (b) example air-mercury successive drainage and imbibition capillary pressure curves.

The observed low mobility of both the wetting and the non-wetting phases leads Cluff & Byrnes (2010) to postulate the “Permeability Jail” concept for explaining typical two-phase (gas-water) relative permeability behaviour in tight gas-sandstone reservoirs. Although the basic behaviour is typical of any two-phase flow system, where one fluid phase interferes with the ability of the other phase to flow freely, the combination of small pore throats in tight gas reservoirs with a reactive, polar, liquid phase (water) leads to unexpected behaviour. The phenomena are observed only in very low-permeability formations, typically with absolute gas permeabilities below

50 micro-Darcies ($< 5E-17 \text{ m}^2$). According to Cluff & Byrnes (2010), the mobility reduction varies by rock type and specifics of the pore geometry, but typically occurs in the rough 55% – 80% S_w range. Tighter rocks tend to have a broader S_w range in “jail”. Jail occurs because water is tightly held by capillary forces in the small pore throats of a tight gas sandstone, blocking the flow of gas through those throats, while at the same time the amount of free water connected through those same throats is extremely low and discontinuous over more than a few pore lengths. It is the absence of larger pore throats that are not completely blocked by pendular water that prevents the flow of gas through a rock in “jail”.

Gas entry pressure – permeability relationships

In petroleum engineering, the gas transport capacity of rock formations is often expressed in terms of gas-entry pressure – permeability relationships. The gas-entry pressure is usually derived from mercury-intrusion porosimetry whereas permeabilities are derived from gas-permeation experiments on dried samples. Corrections are made for slip flow of the compressible gas (Klinkenberg correction). A survey of databases from different lithologies is given in the following section.

In the framework of the Mesaverde Tight Gas Sandstones project, Byrnes et al. (2009) cross-plotted a comprehensive data set of lithic sandstones and gas shales (Fig. 3-59) and derived a characteristic power law relationship for the investigated formations:

$$P_{te}[psia] = 8.6 \cdot k^{-0.42}[mD] \text{ respectively } P_{te}[Pa] = 0.026 \cdot k^{-0.42}[m^2]$$

Similar power law relationships have been derived for other lithologies. Davies (1991) compiled the results of two-phase flow laboratory experiments for shales, sandstones, anhydrites and carbonates in New Mexico and derived a functional relationship between the gas-threshold pressure and the intrinsic permeability of the test samples:

$$P_{te}[Pa] = 0.56 \cdot k^{0.3462}[m^2]$$

Ibrahim et al. (1970) and Ingram et al. (1997) compiled oil industry data on the threshold capillary displacement pressure of low-permeability rocks (see Fig. 3-59b), suggesting that the required gas pressure is often so large that it can approach the lithostatic stress (see also Horseman 2001). Their dataset has been matched manually to the power law relationship with the following coefficients:

$$P_{te}[Pa] = 6.0 \cdot k^{0.333}[m^2]$$

Pusch et al. (2006) provide a relationship for the low-permeability Rotliegend sandstones in Northern Germany:

$$P_{te}[MPa] = 10.6 \cdot k^{0.6932}[mD] \text{ respectively } P_{te}[Pa] = 4.E-6 \cdot k^{0.693}[m^2]$$

The datasets by Byrnes et al. (2009), Davies (1991) and Pusch et al. (2006) suggest that consistent and reliable relationships can be established for a given geological setting when the studied rock formations exhibit a comparable mineralogical and lithological composition. However, the comparison of different entry pressure – permeability relationships shown in Fig. 3-60 displays a

huge spread, revealing a strong dependence of the entry pressures on mineralogy, lithology and other site-specific characteristics such as burial depth. It can be concluded that the transferability of such empirical relationships is limited and cannot substitute site-specific data compilations.

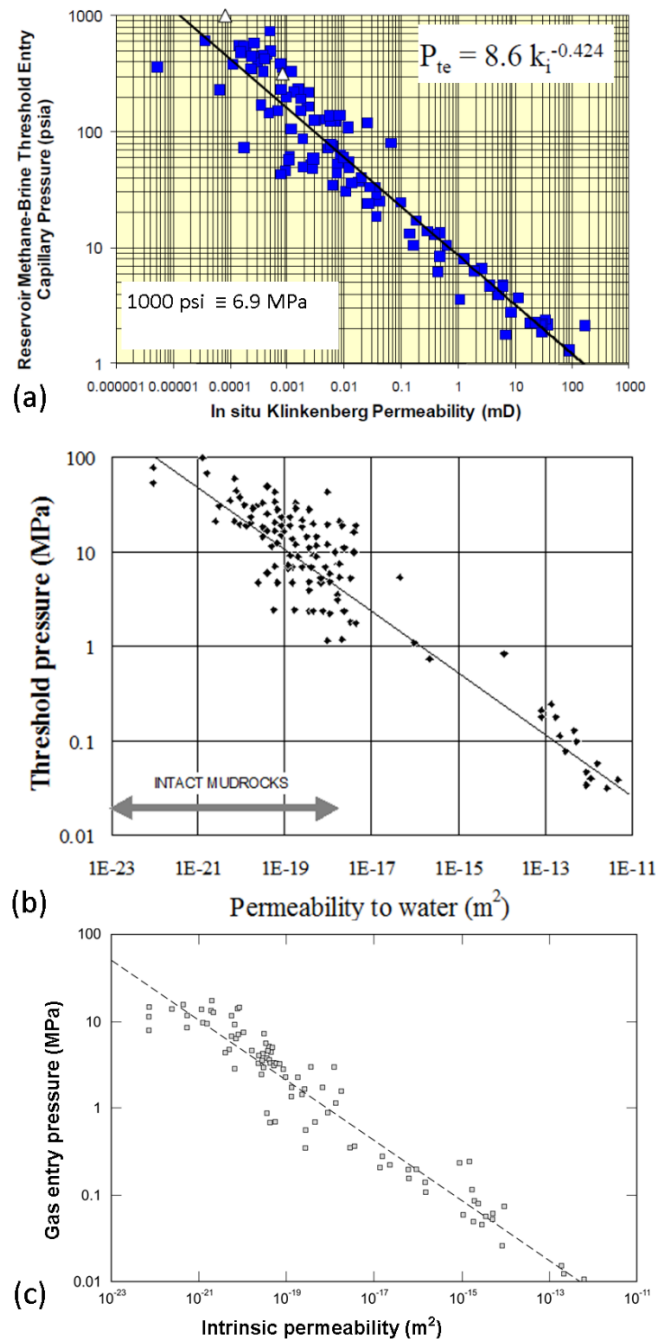


Fig. 3-59: Empirical threshold entry pressure – permeability relationships for various lithologies

(a) Lithic sandstones (blue squares) and gas shales (open triangles) collected within the Mesaverde Tight Gas Sandstones project (from Byrnes et al. 2009); (b) wide range of undifferentiated lithologies, including shale, limestone and anhydrite, based on in-situ measurements (from: Ibrahim et al. 1970; Ingram et al. 1997); (c) shales, sandstones, anhydrites and carbonates in New Mexico (from Davies 1991).

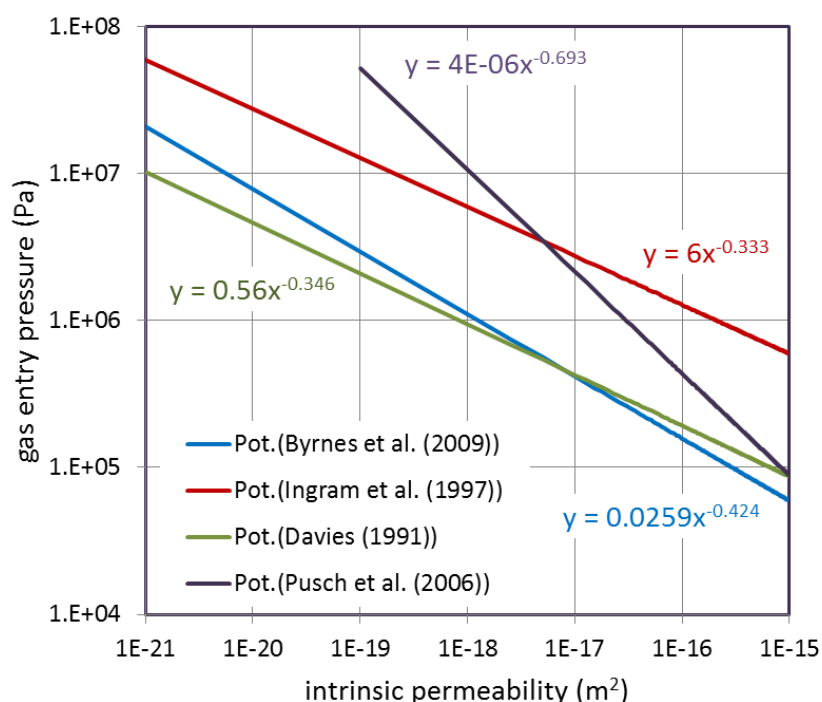


Fig. 3-60: Comparison of entry pressure – permeability relationships from different lithologies and different geological settings

(From Byrnes et al. 2009, Ingram et al. 1997, Davies 1991, Pusch et al. 2006).

3.4.5 Hydrogen adsorption

Hydrogen uptake by clay minerals

Clay minerals, despite their natural abundance, large surface area and good sorption capacities, have not been extensively studied for hydrogen storage. The intercalation of H₂ in interlayer spaces and micropores between clay particles is facilitated by a strong electrostatic field, favourable interlayer space geometry, and a micropore network close to the kinetic diameter of hydrogen (2.89 Å).

Studies on hydrogen sorption in clay-rich media have primarily focused on high-level radioactive waste disposal scenarios. Hydrogen, a product of anoxic corrosion and water radiolysis, can affect repository barrier integrity if its generation exceeds clay-sorption capacity. Difficulties in conducting experiments on natural clays and clay rock include leakage-prone setups and microbial interference (Vinsot et al. 2014, Jacops et al. 2015, Bagnoud et al. 2016).

Pioneering studies on Callovo-Oxfordian claystone and montmorillonite reveal that dry montmorillonite can adsorb up to 0.2 wt.% H₂ at 30 bar H₂ pressure and 90 °C (Didier 2012, Didier et al. 2012, Bardelli et al. 2014, Mondelli et al. 2015). Despite being less studied than metal organic frameworks (MOFs), clay minerals show promising storage capacities comparable to MOFs but are significantly less expensive (Edge et al. 2014).

Hydrogen sorption onto dry clay rock reaches approximately 0.1% in weight, similar to methane and CO₂ sorption (Bardelli et al. 2014, Didier et al. 2012). However, water saturation diminishes H₂ sorption effects. Neutron-scattering studies reveal the structure and dynamics of hydrogen physisorbed in the interlayer space of montmorillonite and laponite (Bardelli et al. 2014, Mondelli et al. 2015, Edge et al. 2014), showing slower diffusion compared to bulk liquid water (Edge et al. 2014).

Molecular sorption of H₂ onto clay aggregates is recognised as a retardation mechanism, contributing to the long-term safety functions of clayey barrier materials. This reduces gas pressure build-up and retards the transport of volatile radionuclides in the free gas phase.

Hydrogen adsorption on claystone at room temperature and moderate pressure can reach up to 0.1 wt.% (Didier 2012, Bardelli et al. 2014). However, compared to MOFs, activated carbon, or zeolite materials (Voskuilen et al. 2012), these measurements appear surprisingly high. Hydrogen uptake by COx claystone is slightly enhanced at 90 °C when compared to 25 °C, contrary to general expectations based on gas adsorption on porous materials (Bardelli et al. 2014).

The available data on H₂ adsorption on natural claystone are insufficient for a robust assessment. There is a need for a robust protocol for H₂ isotherm measurements considering temperature, pressure and relative humidity. The contribution of claystone organic content to H₂ uptake also requires evaluation. While molecular sorption has been historically neglected in repository performance assessments, understanding H₂ sorption and its consequences is crucial, especially for repository concepts vulnerable to gas-pressure build-up scenarios.

Hydrogen production from corrosion of metals in the deep geological repository occurs under anaerobic conditions, which typically starts after closure of the underground tunnels, SF/HLW emplacement drifts and L/ILW emplacement caverns. Maintaining aerobic conditions after backfilling a spent fuel emplacement drift is thus important for canister material selection and design, and for predicting hydrogen production onset. Giroud et al. (2018) studied O₂ monitoring results during the Full-Scale Emplacement Experiment at the Mont Terri URL (Müller et al. 2017). The monitoring indicated the disappearance of gaseous O₂ and the onset of anaerobic conditions shortly after backfilling, even before drift closure for the deepest sections. Laboratory experiments reveal significant O₂ adsorption on granular bentonite at high temperatures and, in principle, at lower temperatures and humidity (Giroud et al. 2018). Gas sorption on bentonite needs consideration in the O₂ balance. Results suggest that anaerobic conditions can be reached within weeks to a few months after drift closure for spent fuel, contrasting earlier estimates of aerobic conditions lasting from a few years to several decades.

Lessons learned from solid-state H₂ storage

Hydrogen adsorption (physisorption) on various materials has been primarily examined in the context of solid-state hydrogen storage, studying various key materials, which include (Voskuilen et al. 2012):

1. MOFs: These crystalline compounds consist of metal ions coordinated to a rigid structure of organic molecules, forming a microporous structure (Lee et al. 2007, Vitillo et al. 2008, Hirscher et al. 2010). MOFs are the most studied and promising materials for hydrogen storage, with some capable of storing up to 7.5 wt.% at 77 K (Wong-Foy et al. 2006).
2. Zeolites: Crystallised aluminosilicates characterised by a microporous structure, zeolites have pore volumes close to the kinetic diameter of molecular hydrogen. They exhibit increased trapping capacity, storing up to 1.5 wt.% H₂ at 77 K (Palomino et al. 2006, Ramirez-Cuesta & Mitchell 2007).

3. Nanotubes (Kadono et al. 2003, Patchkovskii et al. 2005) and carbon nanofibres (Marella & Tomaselli 2006) offer advantages such as low densities, high chemical stabilities, and good sorption capacities (ranging from 1.4 to 6.8 wt.% H₂ at 77 K) based on manufacturing processes.

These materials can be functionalised to enhance H₂ storage capacity. For example, “open metal site”-MOFs, designed with transition metal ions in their frameworks, are effective in capturing hydrogen molecules inside cavities (Langmi et al. 2014, Gygi et al. 2016).

Additionally, hydrogen can be stored through chemisorption, with metal hydrides (e.g., LaNi₅, MgH₂, LiH, NaAlH₄) offering high-volume capacity and good compactness (Freni et al. 2009, Sakintuna et al. 2007). Metal hydrides store hydrogen directly into their crystal structure through chemisorption, requiring high temperatures (>300 °C) for the absorption process. Some hydrides such as NaAlH₄ have favourable storage decomposition conditions: at 1 bar and at 100 °C, they release up to 5.5 wt.% of hydrogen.

Despite their potential, these materials have significant disadvantages, including high production costs, complex manufacturing processes, low stability (especially MOFs in the presence of water), ease of release of physisorbed hydrogen and potential toxicity. Materials based on physisorption also exhibit a drastic loss of storage capacity as temperature increases from 77 K due to the low enthalpy of H₂ sorption.

4 Gas-related properties of EBS components

4.1 Bentonite

Bentonite and sand/bentonite mixtures are preferred barrier materials due to their low hydraulic conductivity when fully saturated (e.g., Leupin et al. 2016, Jenni et al. 2019), which ensures that solute diffusion, especially of radionuclides, is the primary transport mechanism through the barriers. Bentonite's ability to swell in contact with water is advantageous, as it closes gaps and exerts swelling pressure when mechanically confined.

Various forms of compacted bentonite (e.g., granular, blocks, and sand-mixed) are considered for different functions in the Swiss repository concept. Based on their intended application purpose, selection criteria for bentonite include quality, availability, production techniques, dry grain size, exchangeable ions and accessory minerals.

There are different types of bentonite used by different radioactive waste management organisations. The Swiss disposal concept foresees the use of granular Wyoming sodium bentonite (MX-80) for different purposes, such as a buffer material for spent fuel canister emplacement and for sealing galleries and shafts. The MX-80 (or Wyoming sodium bentonite) is primarily composed of more than 85% Na-smectite clay. Its mineral composition includes 84.9% smectite (montmorillonite), 4.8% muscovite, 3.7% quartz, 5.2% feldspar and 1.3% calcite (Plötze & Weber 2007). The material has a high specific surface area, with 523 m²/g from adsorbed water content and 33.1 m²/g from nitrogen adsorption. It exhibits high values for liquid limit (420%) and plastic limit (65%), indicating its high water activity. The specific gravity is reported as 2.74, and the smectite minerals have a cation-exchange capacity of 74 meq/100 g, including 52.4 meq/100 g sodium, 13.2 meq/100 g magnesium and 1.4 meq/100 g potassium.

Several research groups conducted a comprehensive geotechnical characterisation of this granular Wyoming bentonite (Molinero Guerra et al. 2017, Molinero Guerra et al. 2018, Bernachy-Barbe et al. 2020, Seiphoori 2015), focusing on different grain sizes and mixtures, including unsaturated behaviour under various thermo-hydro-mechanical conditions. Swelling tests were performed to evaluate the bentonite's swelling properties. The findings at both macroscopic and microscopic levels were used to develop a water-retention model that considers hydro-mechanical coupling and microstructural changes.

Fig. 4-1a illustrates the swelling pressure over time at constant volume conditions for granular bentonite with varying dry densities using an optimised Fuller granulometry. Fig. 4-1 shows the results of swelling-pressure measurements in relation to dry density. These align with findings from previous studies by Bucher & Müller-Vonmoos (1989) and Karnland et al. (2008), suggesting consistency with compacted blocks.

The gas-transport capacity of bentonite and sand / bentonite mixtures depends on hydro-mechanical conditions and emplacement procedures. Factors such as the form of the material, emplacement, compaction methods and initial dry density are crucial design parameters. After emplacement, the hydro-mechanical properties, including those affecting gas transport, evolve during the hydration process, which depends on water availability, mobility within the bentonite, mechanical conditions, swelling and pressure exertion.

The swelling capacity of bentonite is notably affected by the salinity of the porewater, as reported in studies by Zhu et al. (2013), Navarro et al. (2017), and Shehata et al. (2020). Bentonite exposed to NaCl or CaCl₂ solutions exhibits lower swelling pressure compared to exposure to distilled water. Consequently, the geochemical environment of the repository, as indicated by Guo & Fall (2021), is expected to influence gas transport in saturated bentonite.

Recent experimental investigations (Section 4.1.1) and modelling activities (Sections 4.1.2 and 4.1.3) on gas transport in bentonite are reviewed in the subsequent paragraphs. The gas-related and thermal-reference properties of granular bentonite and compacted bentonite blocks (Section 4.1.4) are taken from a comprehensive calibration exercise in the context of the In-situ Heater Test in VE Microtunnel (HE-E) at the Mont Terri URL as well as of the Long-term Performance of Engineered Barrier Systems (PEBS) project (Gaus et al. 2014a, Gaus et al. 2014b).

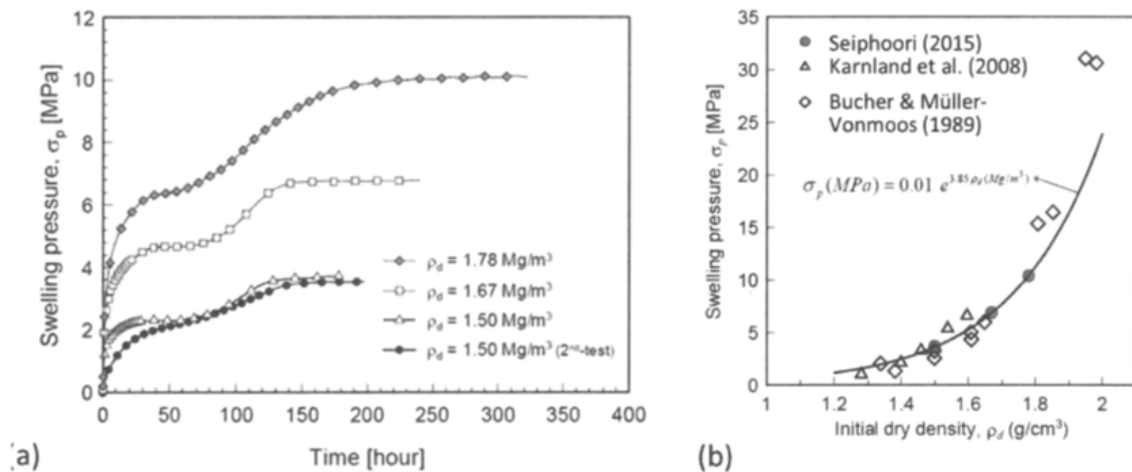


Fig. 4-1: Swelling behaviour of MX-80 granular bentonite

(Modified after Seiphoori 2015).

(a) Swelling pressure developed under constant volume conditions at different dry densities for Wyoming granular bentonite; (b) constant volume swelling pressure.

4.1.1 Gas-related characteristics of MX-80 bentonite

The hydro-mechanical properties of bentonite are greatly influenced by the montmorillonite content. Key properties of saturated samples, such as intrinsic permeability, gas entry value and swelling pressure, are directly controlled by the dry density of the bentonite according to Villar (2005), Seiphoori et al. (2014), Villar et al. (2014), Xu et al. (2017) and Xu et al. (2020). A high dry density results in more expansive clay minerals per unit volume, leading to high swelling pressure when fully saturated under constant volume conditions. The immobile adsorbed water film reduces the porous space available for fluid flow, resulting in very low intrinsic permeability and a high gas-entry value in saturated bentonite with a high dry density.

Unsaturated bentonite has double-pore structures, including inter-aggregate and intra-aggregate pores, resulting in a bimodal pore-size distribution (Gens & Alonso 1992, Alonso et al. 1999, Sanchez et al. 2016, Dieudonné et al. 2017). As bentonite is progressively hydrated under constant volume conditions, inter-aggregate pores gradually reduce due to clay-particle swelling (Gens & Alonso 1992), suggesting that at the saturated state, bentonite primarily presents a unimodal pore-size distribution. Recent mercury-intrusion porosimetry (MIP) results show that saturated bentonite can exhibit a bimodal pore-size distribution, although less pronounced than in as-compacted unsaturated bentonite (Madaschi & Laloui 2018b) (Fig. 4-2).

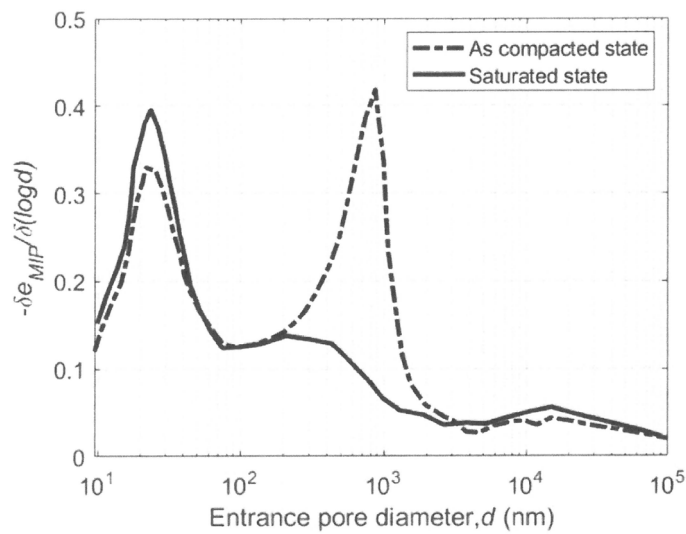


Fig. 4-2: Pore-size distribution of as-compacted and saturated bentonite
(From Guo & Fall 2021 after Madaschi & Laloui 2018a).

The μ -CT images confirm the double-pore structure of saturated bentonite, with fissures between clay grains and pores within grains (Gonzalez-Blanco et al. 2018). Under high gas pressure, these fissures can be activated and serve as preferential gas-flow pathways (Fig. 4-3). The existence of wider passages in highly compacted bentonite is also confirmed in previous studies (Pusch & Forsberg 1983, Pusch & Hökmark 1990, Xu et al. 2017).

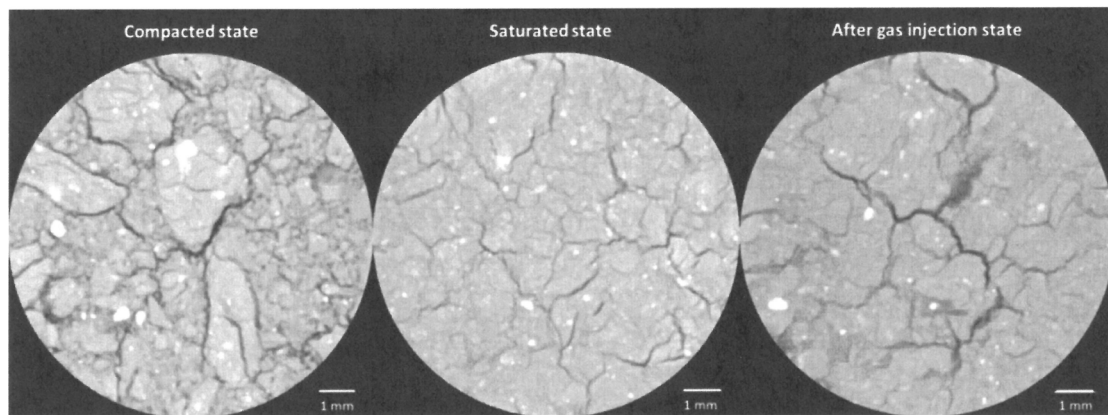


Fig. 4-3: μ -CT images of samples at compacted and saturated states as well as after gas injection
(From Gonzalez-Blanco et al. 2018).

Whether saturated bentonite is considered a porous medium with double-pore structures depends on the context (Guo & Fall 2021). In applications focusing on overall mechanical behaviour, it could be appropriate to consider it a single-porosity medium, as the smaller number of larger pores has no significant influence on mechanical behaviour. In contrast, for research and applications involving highly pressurised gas, the larger connected pores, even if they account for only a small fraction of the total porosity, significantly impact the gas-transport process. These larger connected pores can serve as preferential flow pathways, justifying the consideration of saturated bentonite as a double-porosity medium, with the larger connected pores serving as potential flow pathways while the smaller pores in the matrix remain saturated.

Seiphoori (2015) studied the water-retention curves of MX-80 granular bentonite with dry densities ranging from 1,500 kg/m³ to 1,800 kg/m³ over successive wetting and drying cycles. Gas-entry pressures were derived from these curves, showing a significant increase in gas-entry pressure with higher dry density and decreasing void ratio (Fig. 4-4). Additional tests were performed on samples with a void ratio of 0.53 ($\rho_d = 1.80$ g/cm³), revealing an irreversible modification in water-retention behaviour during the first wetting stage (Fig. 4-5). This change was attributed to alterations in the fabric of the material after saturation, indicated by modifications in pore-size distribution observed in MIP results.

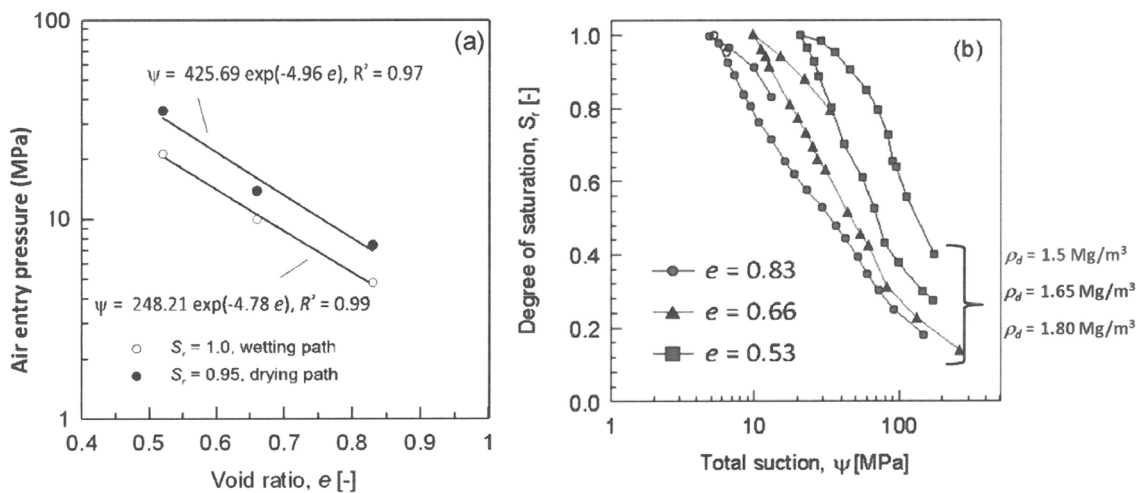


Fig. 4-4: Water-retention behaviour of Wyoming granular bentonite with dry densities between 1,500 kg/m³ and 1,800 kg/m³ under a constant void ratio

(a) Empirical correlation between gas-entry pressure and void ratio (derived from water-retention curves); (b) water-retention curve along a wetting path, followed by a single drying path (Seiphoori 2015).

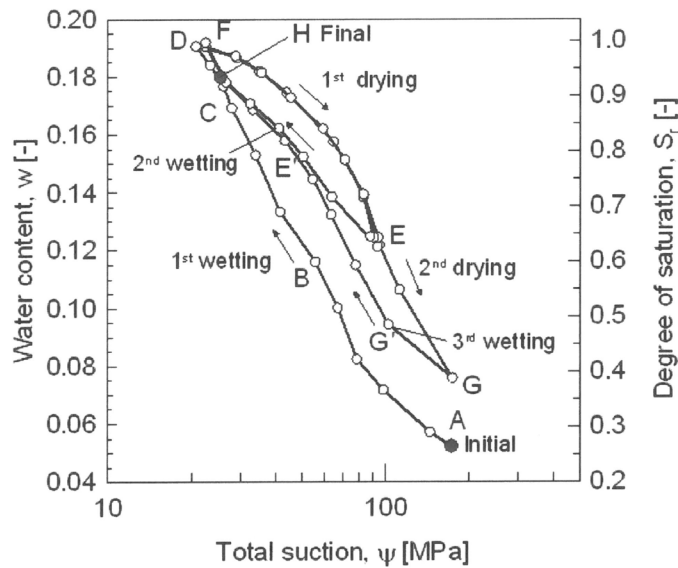


Fig. 4-5: Hysteresis of water-retention behaviour in wetting and drying cycles
(From Seiphoori 2015).

The compacted sample is wetted in steps (Path A – B – C – D) until full saturation is reached (Point D). The main drying path ends at a maximum suction value of 95 MPa (Path D – E). A second wetting path (E – F) is imposed, again reaching full saturation. Drying is then initiated once more until a suction of 174.5 MPa is attained (Point G), succeeded by a final wetting stage until a degree of saturation of 0.95 is reached (Point H).

The water-retention capacity of MX-80 bentonite and its dependence on dry density were analysed by Jacinto et al. (2009) and Pintado et al. (2013). They found that the influence of dry density on water-retention capacity varies with suction levels, with a threshold of around 30 MPa (Fig. 4-6). For suctions above this threshold, higher dry density results in slightly higher water-content retention, while for lower suctions, lower dry density leads to higher water-content retention.

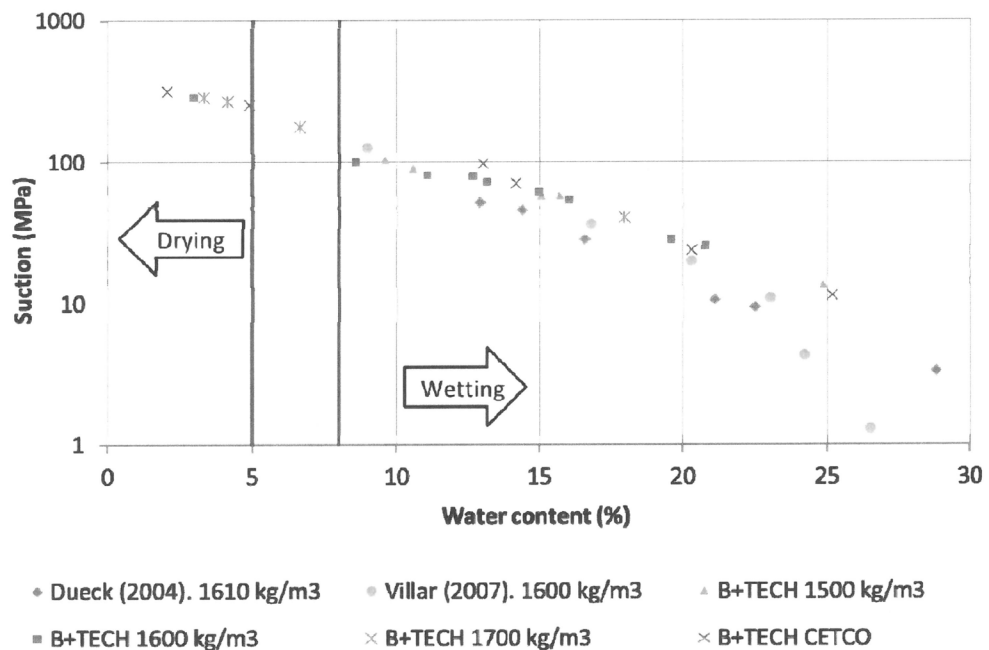


Fig. 4-6: Water-retention curve in terms of water content versus suction of MX-80 samples for different dry-density values

The suction values considered are the average of the psychrometer measurements between the vacuum and the pressure face. The initial water content was between 5 and 8%. The experiments were conducted by B+Tech for both Vo/clay KWK (B+TECH 1,500, 1,600 and 1,700 kg/m³) and Cetco MX-80 bentonites (B+TECH CETCO) and Villar (2007) (1,600 kg/m³) (Pintado et al. 2013).

At the end of Stage 2 of the SGT, Nagra launched a comprehensive laboratory programme to characterise gas- and water-transport properties of compacted bentonite as part of the Äspö Task Force on Engineered Barriers (“EBS Task Force”). The experimental programme was conducted by Romero & Gonzalez-Blanco (2017) and Romero & Gonzalez-Blanco (2019) and formed the basis for a modelling benchmark to improve existing modelling capabilities in the field of THM processes and to develop advanced simulation tools for gas transport in bentonite.

Romero & Gonzalez-Blanco (2019) conducted multiple gas-invasion experiments in compacted granular MX-80 bentonite with dry densities between 1.45 and 1.55 g/cm³ Fig. 4-7). They investigated the impact of grain-size distribution, sample preparation, stress path during hydration on water and gas-permeation results. The tests revealed significant variation in measured water permeabilities, with gas-injection tests conducted using nitrogen and helium at different injection rates. These experiments highlighted that gas-transport processes in compacted bentonite are influenced by various factors, including dry density, grain-size distribution, compaction and hydration processes, and gas injection rates.

The experiments involved a series of oedometer tests that included (1) wetting of the bentonite powder to a desired water content, (2) static compaction to a target dry density (1.55 Mg/m³), (3) elastic loading up to a specified compaction of vertical stress (5 MPa), (4) saturation at constant vertical stress, (5) water-permeability test under controlled-gradient and constant vertical stress, and (6) air-injection tests at constant volumetric injection rates. In addition, micro-structural analyses were performed indicating bi-modal pore-size density (PSD) distributions that changed between the initial as-compacted state, after saturation and after air-injection tests.

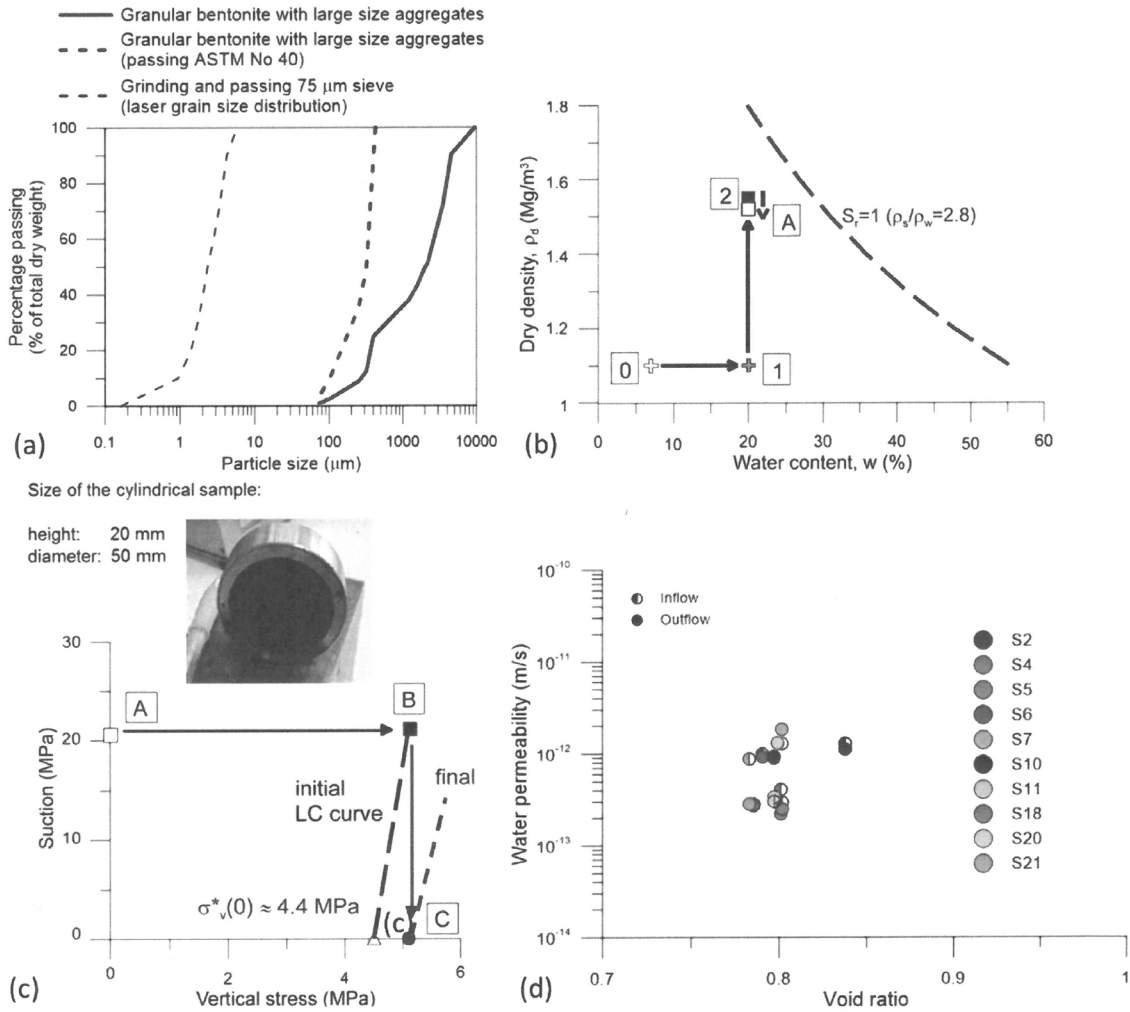


Fig. 4-7: Investigations on the impact of the sample preparation procedure on the results of water-/gas-injection tests with compacted granular bentonite (From Romero & Gonzalez-Blanco 2019).

(a) Grain-size distributions of the tested materials, (b) sample preparation paths to reach a dry density of 1.55 g/cm^3 , (c) stress paths followed under oedometer conditions, (d) water-permeability results (inflow and outflow data) as a function of the void ratio.

A modelling benchmark was established to compare the different approaches for modelling laboratory experiments on gas transport in initially fully saturated bentonite samples along well-defined stress paths. Special attention was given to the deformation occurring along the different hydraulic and gas-injection/-dissipation stages. For this, highly accurate experiments in triaxial and oedometer configurations were required together with detailed analysis of the microstructural changes of the bentonite when subjected to complex stress paths, including wetting stages and gas invasion (Romero & Gonzalez-Blanco 2017, Romero & Gonzalez-Blanco 2019).

Fig. 4-8 shows (a) the test configuration of a helium-injection test for Sample S18; (b) the measured injection pressure, outflow volume at the downstream boundary at a fixed outflow pressure, and the average axial strain calculated based on the recorded axial displacement at the top of the sample; and (c) is a plot of axial strain versus constitutive stress (vertical stress minus gas pressure at the upstream boundary). The applied vertical stress was 5 MPa and initial pressure of the fully saturated sample was 0.5 MPa.

The gas pressure at the upstream boundary increased from 0.5 (Point A in Fig. 4-8b) to 4 MPa (Point B in Fig. 4-8b), subject to a constant volumetric helium-injection rate of 100 mL/min, while the sample expansion and outflow were insignificant. After shut-in, the sample started to expand to a maximum (Point B') while the pressure only showed a small gradual decline (Fig. 4-8b). Following this (Point B'), the outflow rate increased significantly while the sample started to compress to near initial condition by the end of the test (Point C). This is also indicated in the axial strain evolution (Fig. 4-8c), where the constitutive stress remained largely constant (sample underwent negligible expansion) during the injection phase (Points A to B), followed by an increase in axial strain and corresponding porosity changes, as the gas-pressure front propagates into the sample (Points B to B'), associated with a slight decrease in the injection pressure and corresponding small increase in the constitutive stress. After peak strain (Point B'), the outflow rate increased and the injection pressure started to decline (from Points B' to C), resulting in the compression of the sample and a corresponding increase in the constitutive stress.

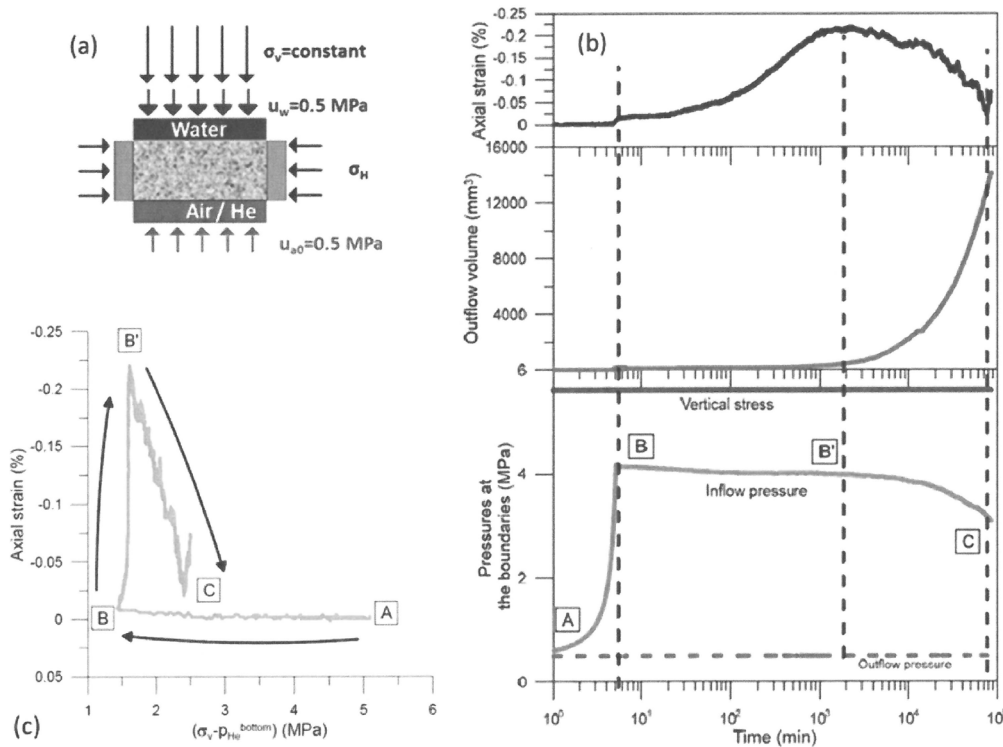


Fig. 4-8: Gas-injection test on Sample S18 with helium at a volumetric flow rate of 100 mL/min

(From Romero & Gonzalez-Blanco 2019).

(a) Schematics of test configuration with the hydraulic and mechanical initial/boundary conditions; (b) time evolution of pressures at the boundaries, outflow volume and axial deformation of the sample; (c) axial strain versus constitutive stress (vertical stress minus He pressure at the upstream boundary).

4.1.2 Modelling assessment and valuation strategies

Three modelling teams participated in the evaluation of different approaches for modelling the laboratory experiments on gas transport in initially fully saturated bentonite samples along well-defined stress paths: EPFL, UPC and INTERA. Three numerical simulators were involved: Code_Bright, developed at UPC (Olivella et al. 1994, Gens & Olivella 2001), used by CIMNE-UPC; Lagamine, developed at ULG (Collin 2003, Gerard et al. 2008), used by EPFL; and the TOUGH2 family, developed at Lawrence Berkeley National Laboratory (Pruess et al. 1999, Finsterle 2007) and used by INTERA.

Both Lagamine and Code_Bright are thermo-hydro-mechanical fully coupled, finite element codes. In this particular study, the application of both codes focused on simulations of water and gas flow in deformable porous media for assessment of gas flow in bentonite. The theoretical hydromechanical frameworks are similar and are composed of two main balance equations: i) mass balances for water and gas; and ii) momentum-balance equation for mechanical equilibrium. The hydromechanical coupling is mainly based on the effective stress concept (i.e., the difference between total mechanical stresses and gas and/or water pressures).

TOUGH2, which belongs to the TOUGH family suite of software codes, is an integrated finite difference code for simulating the transport of heat, water and gas in porous media. In TOUGH2's formulation, the pore-compressibility concept accounts for volume change per unit of pressure change. A clear preference is noted that the compositional approach was employed by all the three codes for its advantage of writing the mass-balance equation for two-phase fluids in a straightforward manner (Panday & Corapcioglu 1989). The three codes have been extensively used and benchmarked (e.g., Sanchez et al. 2016, Dupray et al. 2013, Papafotiou et al. 2018 and citations within). It is therefore considered that the mathematical formulation and implementation of flow models and constitutive models are verified and validated in the application related to the release of gases from deep geological repositories.

Different approaches and strategies have been adopted by the modelling teams to simulate the gas-flow process in the bentonite. The model conceptualisation can be grouped into two main categories: homogenous and heterogeneous mediums. Both EPFL and UPC simulate the bentonite as a single homogenous medium model. EPFL adopts specific constitutive models to approximate the double structure of bentonite, while UPC introduces an explicit predefined fracture to mimic the gas pathway. Explicitly focusing on the heterogeneity of bentonite, UPC also assessed models with one randomly distributed porosity field and with one statistically based porosity field. Similar to UPC, INTERA assessed the effects of the material's heterogeneity on the behaviour of the bentonite in response to the gas injection, with both statistically based porosity distribution and microstructure-correlated distribution of porosity and the permeability field. In addition to random porosity fields, a structured porosity field was generated from backscatter electron (BSE) images (Keller et al. 2014, Keller et al. 2015) that indicated a network of connected pores (Senger et al. 2018b). In addition to a single medium, INTERA's effort included a dual-medium model, which explicitly accounts for the hydromechanical interaction between micro- and macropores of the bentonite, as described below.

Uncertainty quantification of the models is addressed in detail, including parameter sensibility analysis (UPC), Monte Carlo analysis (EPFL, INTERA), inverse modelling (INTERA) and Bayesian Maximum A Posteriori estimation and optimisation (EPFL). These tools provided rigorous assessment of the modelling uncertainties and identification of the optimum modelling parameter set.

4.1.3 Model concept and dual-medium implementation

The conceptual model characterising the different PSD behaviours distinguishes a micro-/mesopore domain (D_m) and a macropore domain (D_M) of the bentonite (Fig. 4-9). The macropores collapse during hydration at a nearly constant soil volume (expansion of the D_m at the expense of the D_M). Macropores reopen with gas injection, resulting in a shift of the D_M peak to larger pore sizes. The D_m and D_M domains are assumed to be hydraulically connected, allowing water and potential air flow due to hydraulic and capillary gradients. Changes in the porosity of the D_m and D_M combine to reflect the total deformation of the medium, controlled by the imposed total stress and corresponding effective stress during the different test procedures subject to changing pressure conditions.

The conceptual model was implemented into a numerical model using the MINC concept in TOUGH2 (Pruess et al. 1999) and is described in Senger et al. (2018b). For this, the PSDs were used to develop stochastic fields of the pore sizes for the D_m and D_M domains that were converted to porosity and permeability fields for connected two-dimensional model domains corresponding to the diameter and height of the core sample. The D_M and D_m volumes were based on the ratio of the cumulative PSDs of the “saturated” and “compacted” PSDs.

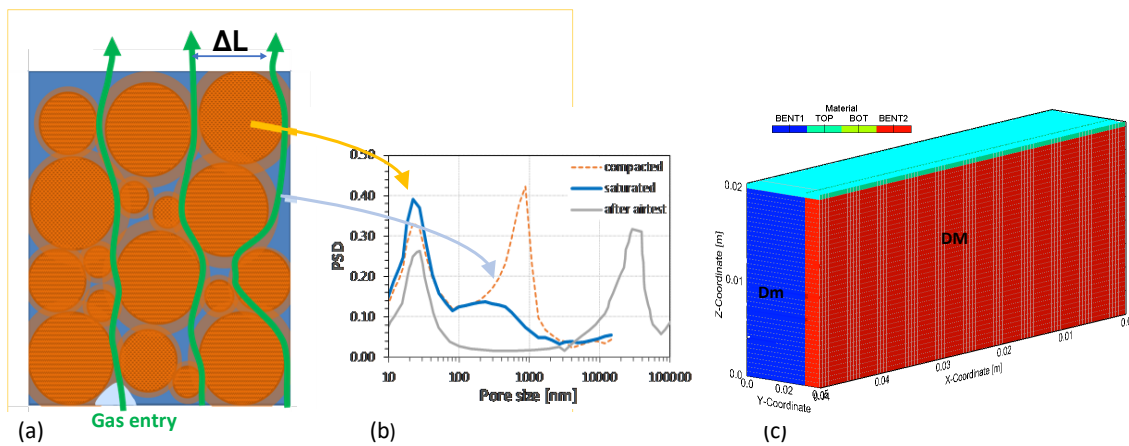


Fig. 4-9: Conceptual representation of MX-80 bentonite in the MINC concept (TOUGH2)

(a) Distinguishing meso-/micropore (D_m) and macropore (D_M) domains that are related to (b) pore-size distributions for the different conditions (i.e., as-compacted, saturated, after air injection); (c) model implementation.

The changes in axial displacement of the core were implemented by assuming an elastic porosity change due to (a) pore compressibility and (b) a non-linear response to effective stress changes. In both cases, the changes in porosity are coupled to changes in permeability and capillary air-entry pressure using constitutive relationships based on either measurements or calibrations to the measured pressures and axial deformation.

In TOUGH2, the effect of pore compressibility C_p is accounted for by the change in porosity ($d\phi$) in response to a change in pressure (dP) according to Eq. 3-1.

Alternatively, the potential changes in porosity can be described as a function of effective stress, using an empirical function developed by Rutqvist et al. (2002) as given in Eq. 3-2, where ϕ_0 is the porosity at zero effective stress, ϕ_r is the residual porosity at high effective stress, and the exponent (α) is a rock parameter that can be used to represent elastic behaviour ($\alpha = 1$) and non-elastic behaviour ($\alpha < 1$).

The modelling of the experiments examined the effective media representations of the D_M and D_m portions of the bentonite, accounting for the change in porosity as a function of pore compressibility due to the change in pressure. This corresponds to an equivalent change in effective stress as the imposed vertical stress is constant. The coupling of the porosity change to permeability and the corresponding change to capillary pressure using Leverett scaling were assumed only for the macropore domain (D_M). An interface zone was implemented to allow scaling of the interface area between the D_M and D_m , and an enhancement factor for gas-relative permeability in the D_M . The calibrated parameters for the different D_M , D_m , interface are summarised in Tab. 4-1.

Tab. 4-1: Implementation of a double-structure representation of MX-80 bentonite in the TOUGH2 code (MINC concept): overview of input parameters

Parameter	Value	Unit
$k(D_m)$	2.50E-20	m^2
$k(D_M)$	1.00E-19	m^2
$C_p(D_m)$	3.00E-09	1/Pa
$C_p(D_M)$	5.00E-10	1/Pa
$vG-P_0(D_m)$	5.00E+07	Pa
$vG-P_0(D_M)$	1.00E+07	Pa
$vG-P_0(BINT)$	7.00E+06	Pa
$k_{por}(D_M)$	20	
$k_{g-fact}(D_M)$	10	
Interface-area-factor	2	

The results in Fig. 4-10a show the simulated injection and outflow pressures, computed axial strain and outflow volumes. Fig. 4-10b shows spatial plots in a vertical cross-section through the bentonite domains D_m (left) and D_M (right) at different times.

The He-injection phase was represented by a prescribed constant injection rate at the inflow chamber. The simulated pressures show good agreement with the measured pressures during the short injection phase and following shut-in (Fig. 4-10a). The axial strain computed from the porosity change also showed good agreement except for the latetime when the measured strain indicated a nearly full recovery. The measured outflow volume was converted to the equivalent He mass accumulation at the constant pressure in the outflow chamber, which compared reasonably well with the simulated He outflow from the D_M . The simulation indicated some water displacement from the D_M , while the outflow from the D_m was negligible.

The spatial distribution of gas saturation and pressures after 5.2 minutes (shut-in) indicated some gas entering the sample in the D_M with pressure increase propagating farther into the D_M (Fig. 4-10b). After 50 minutes, simulated changes in porosity and permeability indicated a small porosity increase in the D_M with a greater increase in permeability. Compared to the axial strain, these results indicate that the early increase in strain occurs only in the D_M . After 1,000 minutes, the D_m showed a significant increase in porosity, whereas the porosity in the D_M did not significantly change. However, the permeability in the D_M remained relatively high, while the D_m showed little change in permeability. This indicates that the expansion of the D_m accounts for much of the measured axial strain.

The pressure increase in the D_M results in water flow from the D_M to the D_m , enhanced by the capillary gradient between the D_M and D_m . This is due to a very low gas saturation (less than 1%) appearing in the D_m based on the van Genuchten capillary pressure curve, which is assumed to have a much greater capillary strength compared to that in the D_M .

The computed axial strain at a later time reflects the magnitude of the pressure recovery, underpredicting the observed compression of the sample (Fig. 4-10a); this suggests non-elastic or hysteretic behaviour.

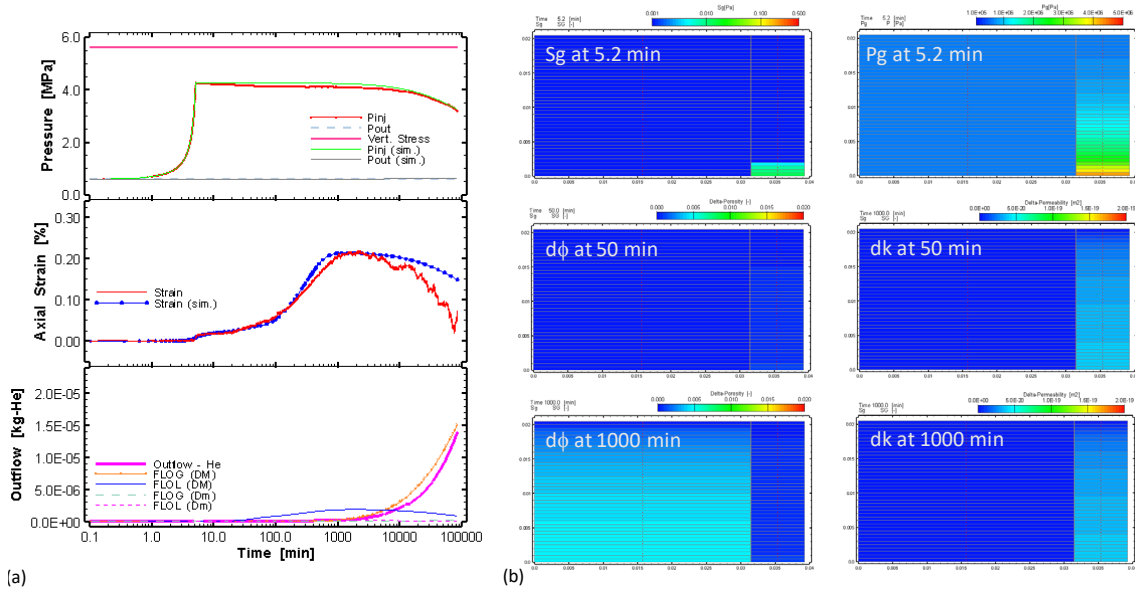


Fig. 4-10: Simulation results of the He-injection test S18

(a) Injection and outflow pressures (top), the axial strain of the combined DM and Dm (middle), outflow volumes (bottom); and (b) spatial plots of gas saturation and pressure after 5.2 minutes (top), change in porosity and permeability after 50 minutes (middle) and after 1,000 minutes (from Senger et al. 2018b).

Further modelling studies examine the potential non-elastic or hysteretic behaviour, and consistency with other gas-injection tests performed as part of the benchmark exercise.

The experimental observations show that the bentonite microstructure and the associated subscale processes significantly determine the gas transport process. The structural features and characteristics can vary depending on the sample preparation / compaction / saturation process. These manifest in significant variations of effective properties used to describe bentonite from the perspective of a representative elementary volume. This has been identified with the modelling efforts of the modelling teams (INTERA, EPFL, UPC) that, despite using different modelling approaches, all concluded that there is no single “best” parameter set to describe the gas process observed in the experiment, but rather a range of uncertainty which is even associated with different parameters introduced in various parameterised models (i.e., pore compressibility, double porosity versus fully coupled models, etc.).

The validation exercises helped to understand the role of experimental uncertainties (e.g., uncertainties arising from sample preparation and dead volume in the test equipment). The exercises also occasioned the call for the further development of numerical models to take into account the dynamics between micro- and macrophases as well as the need for an alternative experimental concept to bracket the time of gas breakthrough to constrain the gas-transport properties at a macroscopic scale.

The three state-of-the-art simulation tools Code_Bright, Lagamine and TOUGH2 were evaluated and used for this task. All are capable of modelling gas and water flow in deformable porous media. Code_Bright and Lagamine share similar frameworks dealing with a fully THM-coupled two-phase flow problem. Both are augmented with constitutive models dedicated to the mechanical behaviour of bentonite undergoing external hydraulic loadings (BBM for UPC, and ACMEG for EPFL). TOUGH2 is a two-phase flow code, but INTERA developed possible effective approaches for pore compressibility to account for the mechanical behaviour of the bentonite.

In addition to the limitations of the different model concepts employed by the different teams, there are shortcomings in the theoretical treatment of two-phase flow in unsaturated media. This includes the potential impact of the dynamic effects associated with capillary pressure saturation relationships, where the capillary pressure depends on the duration of saturation change (Zhuang et al. 2017). Furthermore, new theoretical work on the bentonite provides insight into hydration and the hydromechanical behaviour of bentonite, as described in Bosch et al. (2021); Åkesson et al. (2023).

4.1.4 Reference parameters of MX-80 bentonite

Comprehensive calibrations of thermal properties and two-phase flow properties of bentonite blocks and granular bentonite were carried out in the context of the HE-E experiment at the Mont Terri URL and in the context of the PEBS project (Gaus et al. 2014a, Gaus et al. 2014b). The calibrations served as a basis for the derivation of reference datasets of the thermo-hydraulic properties of granular bentonite/bentonite blocks for model-based assessments of the HLW near-field in Stage 2 of the SGT (Senger et al. 2014a). The same data were used for the model-based assessment of the repository performance in Stage 3 of the SGT (Tab. 4-2).

Tab. 4-2: Hydraulic, two-phase and thermal properties for the different bentonite buffer materials – reference values for model-based performance assessment

(From Senger et al. 2013).

	Symbol, unit	Bentonite blocks	Granular bentonite
Hydraulic and WRC parameters			
Intrinsic permeability	$k [m^2]$	2.5E-21	3.5E-20
Porosity	$\varphi [-]$	0.33	0.33
Compressibility	$\alpha [1/Pa]$	1.0E-9	1.0E-9
$C_p = \alpha/\varphi$	$C_p [1/Pa]$	3.0E-9	3.0E-9
Initial water content	$w_r [%]$	16.5	6.6
Initial saturation	$S_w [-]$	0.5	0.2
Van Genuchten capillary strength ¹	$P_0 [MPa]$	21.9	10
Shape parameter:			
vG-n (kr)	vG-n (kr)	1.42	1.67
vG-n (Pc)	vG-n (Pc)	1.42	1.67
Residual water saturation	$S_{lr} (kr)$ $S_{lr} (Pc)$	0.00 0.01	0.00 0.01
Residual gas saturation	$S_{gr} (kr)$	0.	0.
Thermal parameters			
Density			
• Dry	$\rho [kg/m^3]$	1,806	1,492 / 1,457
• Bulk		1,874 / 1,993	1,581 / 15,431
• Grain		2,700	2,700
Specific heat (dry)	$Cr [J/(kg K)]$	1,058	893
at T = 20 °C		800	856
at T = 110 °C		1,315	1,020
Thermal cond.	$T_c [W/mK]$		
• Dry		0.35	0.35
• Wet		1.30	1.30
Thermal exp.	$T_x [1/ K]$	2.5E-5	2.5E-5

¹ Default value $T_0 = 20\text{ °C}$ for temperature scaling.

4.2 Sand/bentonite (SB) mixtures

For certain engineered barrier components of the L/ILW repository (V1 and V2 seals), a certain gas permeability is desirable to enable the transport of gas from the emplacement caverns at moderate gas overpressures (Nagra 2008). In such cases, sand/bentonite mixtures with relatively low bentonite content are suitable, because they have a low hydraulic conductivity and, at the same time, significant gas permeability. In addition, through the application of appropriate techniques for their emplacement (compaction), their gas-transport properties can be modified to correspond to safety-relevant design requirements. For these reasons, comprehensive research studies have been conducted in the past decades to characterise gas transport in sand/bentonite mixtures (e.g., JAEA 2000, Tashiro et al. 1998, Graham et al. 1997). In particular, a better understanding has been obtained for the microstructure of such mixtures and its importance for gas-transport behaviour. It has been shown that sand/bentonite mixtures with a moderate bentonite content of 20 – 30% are characterised by a multi-modal pore-size distribution (Olson 1969, Collins & McGown 1974, Alonso et al. 1987, Gens & Alonso 1992, Hoffmann et al. 2007). The form of the pore-size distribution depends on a variety of factors, e.g., the degree of compaction and the water content of the sand/bentonite mixture (Nagra 2008). This explains the ability to design these materials in order to exhibit desired properties.

In the Swiss concept for deep geological disposal, S/B mixtures with low bentonite content (typically 20%) are considered suitable sealing and backfilling materials for underground structures, forming the “engineered gas transport system” (EGTS) of the L/ILW repository (Nagra 2008). The EGTS aims to improve gas transport in underground structures without compromising radionuclide retention.

Understanding hydro-mechanical and chemical (HMC) phenomena in 80/20 S/B mixtures is crucial for repository safety. A comprehensive research programme has investigated these mixtures at both macroscopic and microscopic levels. The material comprises quartz sand and MX-80 bentonite in a dry mass ratio of 80/20. The quartz sand’s high chemical and mechanical stability and its role in load support enhances macroscopic mechanical stability and reduces shrinkage, decreasing the risk of fracturing compared to that of pure bentonite.

Index tests by Manca (2016) show the dependence of index properties on water composition (Fig. 4-11). The liquid limit decreases with increasing osmotic suction of water used for testing, while the plastic limit is only slightly affected by water composition. Higher porewater salinity reduces the mixture’s activity, indicating a reduction in the swelling capacity of the bentonite fraction due to the lower swelling capacity of smectite minerals at the particle level. The presence of sand grains in the mixture contributes to the relatively low liquid and plastic limits compared to those of pure bentonite.

Manca (2016) reported additional index properties for the material, including a specific surface area of 105 m²/g and a specific gravity of 2.67. The grain-size distributions are presented in Fig. 4-12.

Dynamic compaction tests were conducted to determine the maximum achievable compaction density for a specific compaction energy. The results, presented in Fig. 4-13a, revealed an optimum water content of 0.12 and a corresponding maximum dry density of 1.88 g/cm³ for a compaction energy of 3.4 J/cm³. These results are specific to an S/B mixture wetted with distilled water. In an oedometer cell, the material exhibited a compression index (Cc) of 0.45 at the as-compacted state and a swelling index (Cs) of 0.01, as shown in Fig. 4-13b.

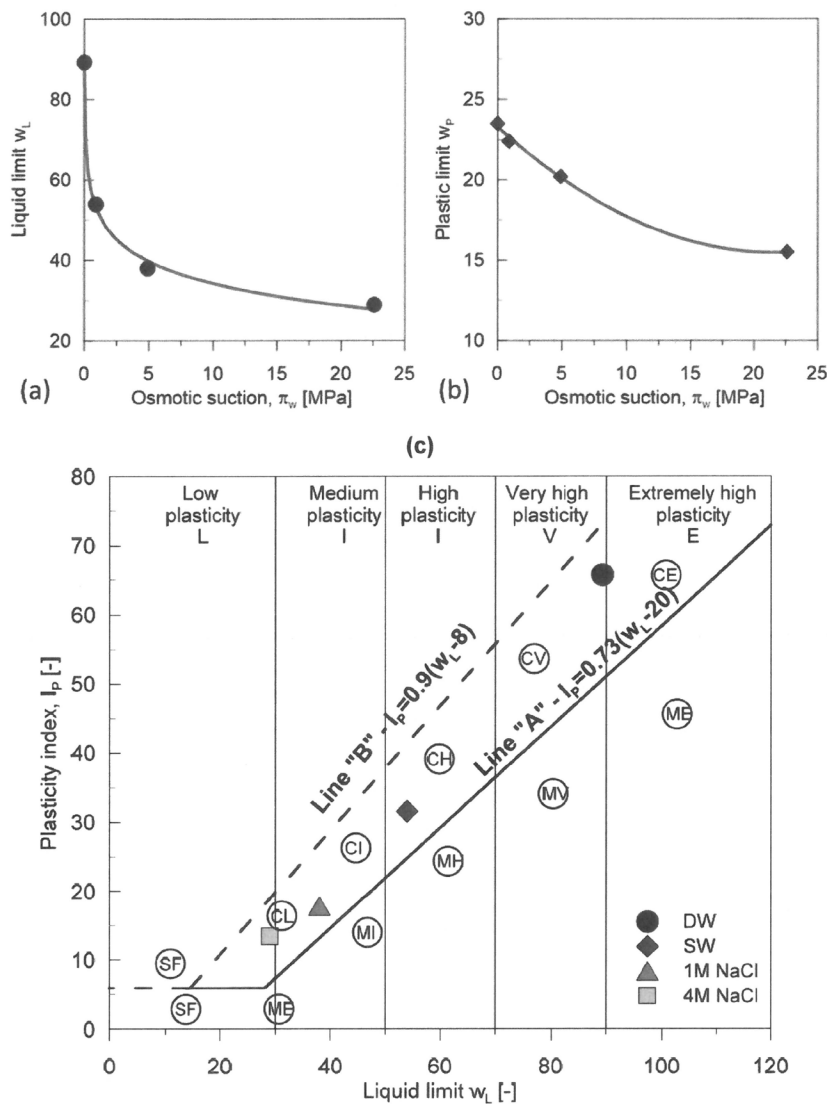


Fig. 4-11: Dependence of the Atterberg limits of 80/20 sand/bentonite mixture on water composition

Modified after Manca (2016).

(a) Decrease of liquid limit and (b) decrease of plastic limit with the increase of osmotic suction of the porewater; (c) plasticity chart. The four different water types are deionised water (DW), synthetic porewater (SW), 1-molar NaCl solution and 4-molar NaCl solution.

Free and constrained swelling tests were conducted in a thick-walled oedometer cell using S/B mixtures with dry densities ranging from 1,300 to 1,800 kg/m³. Deionised water was used for these tests. The swelling strains under free swelling conditions varied from 0.4 to 0.8. Under constant volume conditions, the swelling pressure exhibited a distinct range from 35 kPa ($\rho_d = 1,300$ kg/m³) to 205 kPa ($\rho_d = 1,800$ kg/m³). Transients of swelling strain and swelling pressure can be observed in Fig. 4-14.

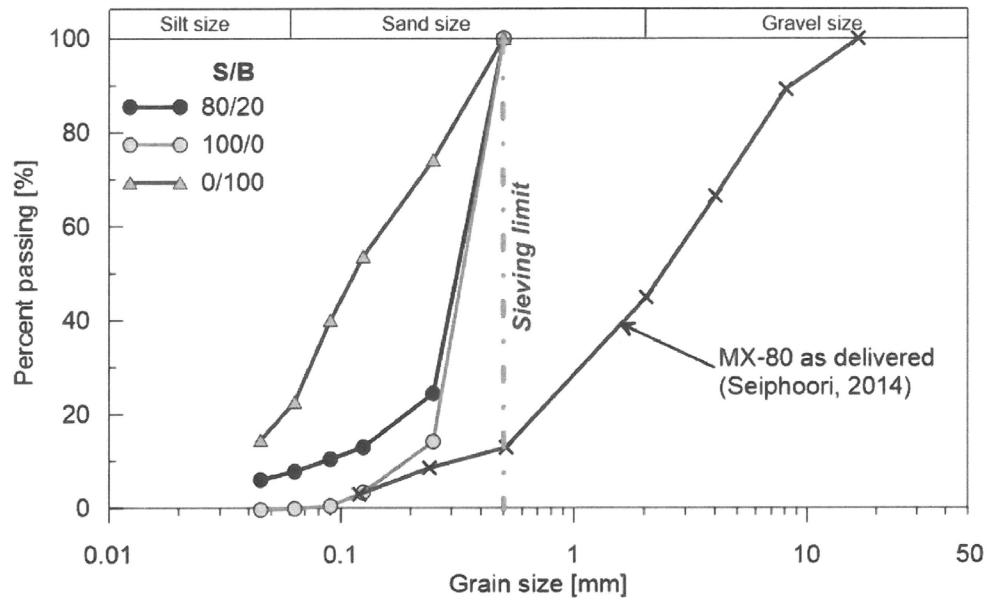


Fig. 4-12: Apparent grain-size distribution of the tested 80/20 sand/bentonite mixture and its two solid components (pure sand and pure bentonite, after sieving to remove the coarse grains)

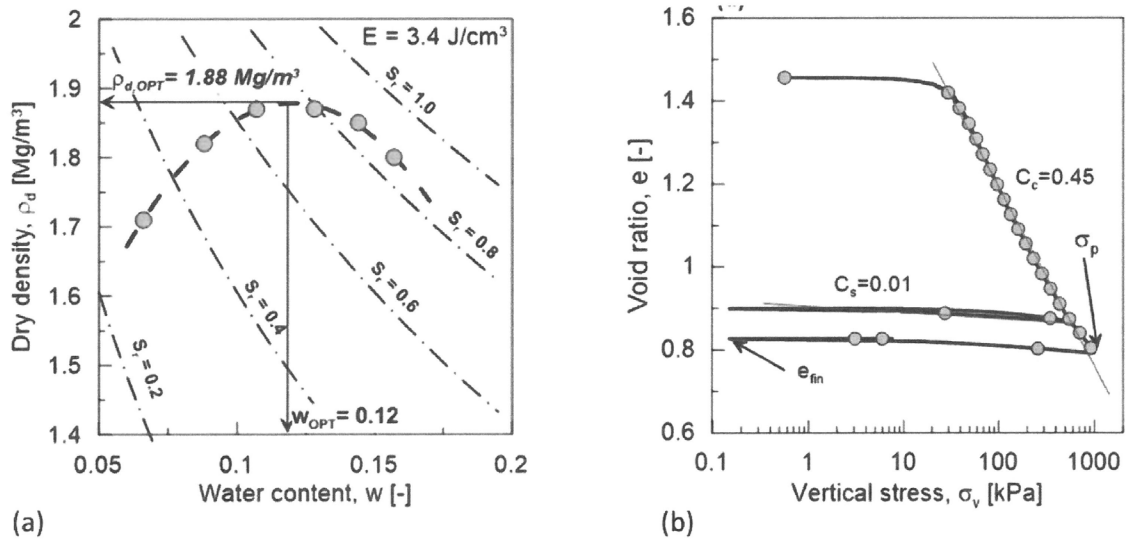


Fig. 4-13: Volumetric behaviour of the 80/20 sand/bentonite mixture

(a) Dynamic compaction test to determine the optimum compaction density, with isolines for saturation degrees; (b) determination of compression and swelling indexes in oedometric configuration.

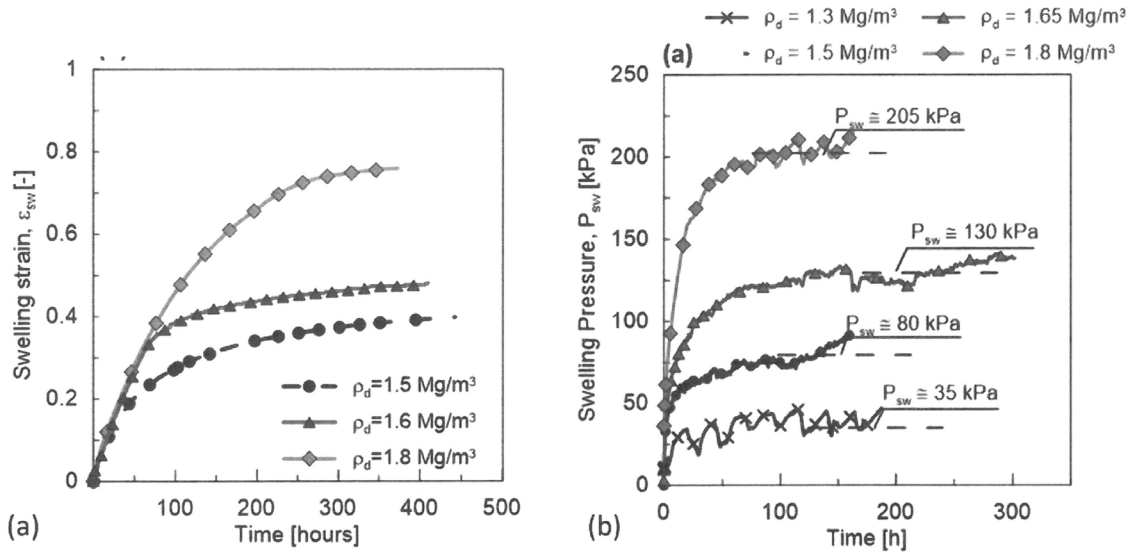


Fig. 4-14: Swelling behaviour of the 80/20 sand/bentonite mixture with dry densities between 1,300 and 1,800 kg/m³

(a) Free swelling strains under oedometric conditions; (b) swelling pressure under constant volume conditions.

4.2.1 Gas-related characteristics of S/B mixture

Manca (2016) studied the geotechnical characteristics of granular S/B (sand/bentonite) mixtures and involved measuring the water-retention behaviour of these mixtures when compacted to dry densities of 1.50 and 1.80 g/cm³. Water-retention curves were obtained using established techniques for suction measurements. The results indicated that S/B mixtures have a lower water-retention capacity compared to pure bentonite, primarily due to the presence of sand and the microstructural characteristics of bentonite (Fig. 4-15).

For total suction above 3 MPa, the water-retention behaviour of S/B mixtures was found to be relatively consistent for both compaction densities, suggesting that compaction density has a minimal effect on water retention (Fig. 4-15). The water appears to be mainly stored in the bentonite fraction's pores, where it is unaffected by compaction, with the dominant retention mechanism being adsorption. In the suction range between 3 and 0.5 MPa, a transitional zone was observed, where both adsorption and capillary-retention mechanisms contributed significantly to total suction. This explains the modest dependency of the mixture's initial matrix and total suctions on dry-density variations. However, for suction below 0.5 MPa, specimens compacted to lower dry densities retained less water due to the larger pore volume.

The study also investigated the evolution of water permeability under partial saturation conditions. Regardless of the initial dry density, the effective permeability of the mixture to the water phase increased with the degree of saturation. This increase was attributed to the expansion of bentonite pores and a greater fraction of pore volume available for water flow. At low degrees of saturation, the water's effective permeability became very small, especially within the smallest pores of the bentonite, where adsorption forces were dominant. This limited water-mobility state was referred to as irreducible or connate-water saturation.

The hydraulic conductivity versus degree of saturation curve displayed hysteresis for both dry densities, with higher hysteresis observed for the specimen compacted to higher dry density and lower void ratio (Fig. 4-16). Additionally, hysteresis was observed in the hydraulic conductivity versus the suction curve, which was associated with irreversible deformation of the internal structure of bentonite during wetting and drying cycles. In summary, the study found that sand/bentonite mixtures allow gas passage at lower pressures while still retaining porewater effectively, making them relevant in visco-capillary flow contexts.

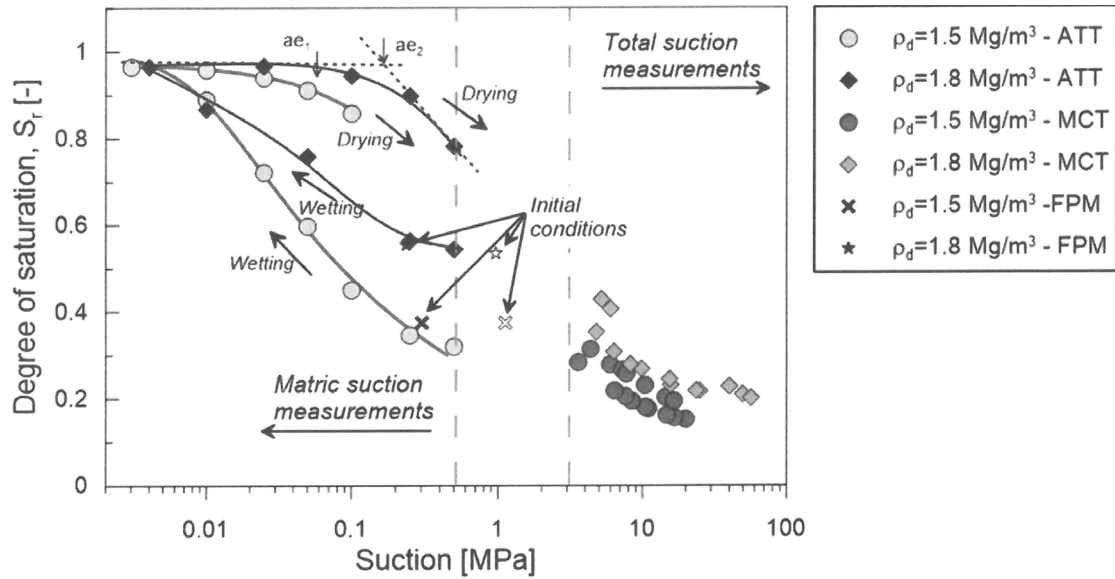


Fig. 4-15: Full-range water-retention curve of the 80/20 sand/bentonite mixture at two different dry densities using well-established techniques for suction measurements

Further details are given in Manca (2016).

FPM = filter-paper method; ATT = axis-translation technique; MCT = microcell technique.

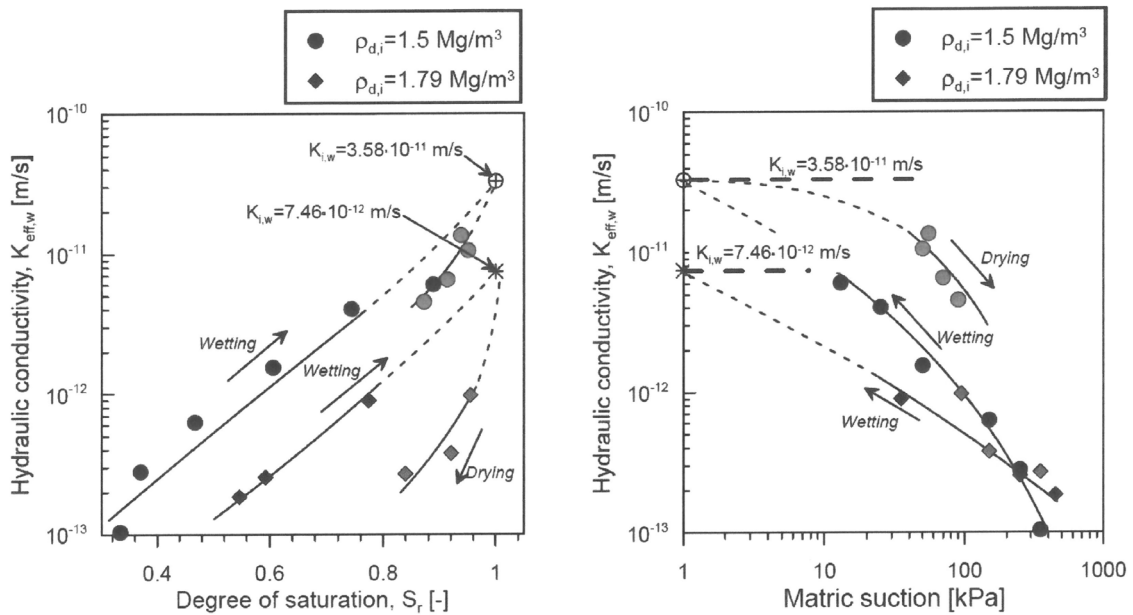


Fig. 4-16: Unsaturated hydraulic conductivity of the sand/bentonite mixture compacted to two different dry densities

(From Manca 2016).

Manca (2016) also performed gas-invasion tests under triaxial conditions to investigate the potential mobilisation of bentonite associated with gas-breakthrough events. The tests were conducted on a fully saturated S/B specimen initially compacted to 1.8 Mg/m^3 . The gas injection resulted in increasing gas pressure up to a peak of 1,038 kPa (Fig. 4-17). A measurable outflow occurred when the gas pressure reached 850 kPa, indicating the displacement of water from the larger pores of the S/B mixture. After the breakthrough event, the gas pressure decreased, reaching a stationary value of approximately 750 kPa, suggesting the maintenance of open gas pathways through the specimen.

During the gas injection, a special device collected bentonite colloids mobilised by the gas phase. Approximately 0.02% of the total dry mass of the specimen (816.63 g) was collected as bentonite particles (Fig. 4-17b), highlighting the likelihood of fine-particle transport in S/B mixtures. The study emphasised the need for further experiments to explore the relationship between the mobilised cumulative mass of bentonite and cumulative gas flow.

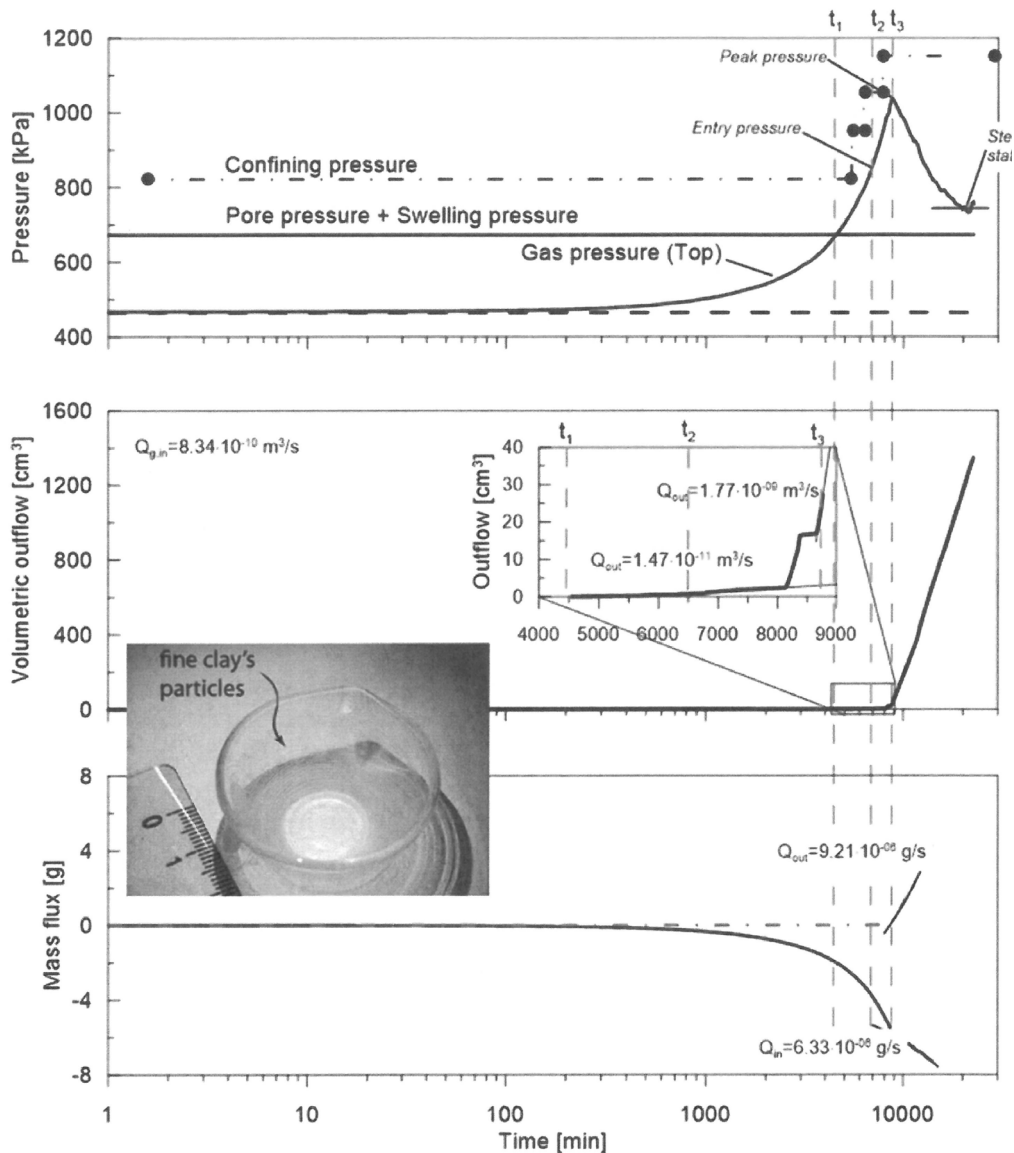


Fig. 4-17: Results of the breakthrough tests on an 80/20 sand/bentonite mixture compacted to 1.8 Mg/m^3

(From Manca 2016).

From top to bottom: evolution of the gas pressure, confining pressure and porewater pressure as well as evolution of the cumulative volumetric outflow and of the cumulative mass flux. The picture shows the mobilised mass during the gas-injection test under constant volume conditions.

The use of a sand/bentonite mixture was also investigated in a field-scale EBS experiment at the Grimsel test site in Switzerland, the so-called Gas Migration Test (GMT) conducted as part of the RD&D programme performed by the Radioactive Waste Management Funding and Research Center (RWMC) of Japan. Hydro-mechanical characterisation was conducted on material from the experiment (Arnedo et al. 2008), and hydraulic- and gas-permeability testing were performed on sand/bentonite mixtures at in-situ compaction densities ranging from 1.50 to 1.85 Mg m^{-3} .

In the study by Kumara et al. (2017), strength and volumetric behaviour of sand/bentonite material subjected to various degree of saturation were investigated. In addition, suction characteristics of specimens before and after loading were studied using a newly available chilled-mirror hygrometer technique (Agus et al. 2010). Cui et al. (2008) focused on the hydraulic characteristics of compacted sand/bentonite mixtures.

Liu et al. (2014a) and Liu et al. (2014b) conducted gas-injection experiments on plugs formed from sand/bentonite mixtures with 70% MX-80 bentonite content. They observed that gas-breakthrough pressures were more sensitive to a sample saturation state than swelling pressure. Gas permeabilities were highly sensitive to water content and applied confining pressure. At a relative humidity of 98%, low gas permeabilities were achieved under in-situ conditions, demonstrating a significant sealing capacity despite incomplete saturation, similar to observations on pure bentonites. Effective gas permeability dropped rapidly when approaching full saturation.

As part of assessing the feasibility of the sealing concepts of underground repository structure using sand/bentonite mixtures, a number of in-situ experiments have been performed in underground rock laboratories (URL), such as the TSX (Tunnel Sealing Experiment) (Martino et al. 2008) and ESP (Enhanced Sealing Project) (Dixon et al. 2014) at Atomic Energy of Canada Limited's (AECL's) URL in Canada, FEBEX (Full-Scale Engineered Barrier Experiment) at the Grimsel Test Site, Switzerland (Huertas et al. 2006), the EB (Engineered Barrier Emplacement Experiment) at the Mont Terri URL, Switzerland (Villar et al. 2014), RESEAL (Repository Sealing) at the Hades URL, Belgium (van Geet et al. 2007) and KEY at the Laboratoire souterrain de Meuse Haute Marne (LSMHM), France (Barnichon, Deleruyelle 2009). In addition, the French Institut de Radioprotection et de Sûreté Nucléaire (IRSN) has conducted the SEALEX (Sealing Performance Experiment) in the Tournemire URL. The Gas-Permeable Seal Test (GAST) experiment at Grimsel represents the seal concept for an L/ILW repository proposed by Nagra as part of the Engineered Gas Transport System (Teodori et al. 2013). More recently, the current German concepts for shaft seals contain the hydraulic sandwich sealing system as a component of the lower seal in host rock implemented in a large-scale experiment at the Mont Terri URL (Wieczorek et al. 2021).

4.2.2 Reference parameters of 80/20 S/B mixture

Hydraulic properties and two-phase flow parameters of 80/20 S/B mixtures can be modified through the application of appropriate techniques for their emplacement (compaction) to correspond to the safety-relevant design requirements (Nagra 2008). The ability to design these materials to exhibit desired properties has been used to optimise the L/ILW repository to enable the transport of gas from the emplacement caverns at moderate gas overpressures (e.g., Papafotiou & Senger 2016). The reference datasets of the two-phase flow parameters of 80/20 S/B mixtures for the model-based assessment of repository performance in Stage 3 of the SGT are given in Tab. 4-3.

Tab. 4-3: Hydraulic and two-phase properties of the 80/20 S/B seal sections V1 and V2 of the L/ILW repository – reference values for model-based assessments of gas release from the L/ILW repository

	Symbol, unit	S/B ¹	Remarks
Hydraulic parameters			
Porosity	ϕ [-]	0.35	From Nagra (2008).
Intrinsic permeability	k [m ²]	5.0E-18	
Pore compressibility	C_p [1/Pa]	1.0E-09	
Initial water content	w_r [%]	18.0	From Nagra (2008).
Initial saturation	S_w [-]	0.50	
Two-phase flow parameters			
van Genuchten capillary strength ²	P_0 [Pa]	4.0E03	
Shape parameter	$vG-n$ (kr) $vG-n$ (Pc)	2.5	
Residual water saturation	S_{lr} (kr) S_{lr} (Pc)	0.30 0.01	
Residual gas saturation	S_{gr} (kr)	0.0	

¹ Only V1-L/ILW and V2-L/ILW; alternative values $n = 1.5$ and $S_{lr}(kr) = 0.05$.

² Default value $T_0 = 20$ °C for temperature scaling.

4.3 Concrete and mortar

Most of the information on concrete and mortar was derived from work done within the Nagra RD&D and associate Swiss researchers at the Swiss Federal Institute of Technology Zürich (Mayer et al. 1992, Mayer & Wittmann 1996, Mayer et al. 1999) and recent French studies, which were compiled in Appendix A of Nagra (2008). The main results are summarised in the following, augmented by studies on cementitious materials used at U.S. Department of Energy disposal facilities.

Normal concretes and mortars are specified for engineering purposes and waste packaging. Concrete composition includes cement (typically Ordinary Portland Cement (OPC)), aggregate (e.g., sand or gravel), water, chemical additives (e.g. retardants, superplasticisers, corrosion inhibitors) and mineral additives (e.g., fly ash, slag, silica fume). Porosities are influenced by the water-cement mixing ratio (w/c) and curing process. Porosity in normal concretes is around 15% for w/c ratios of 0.4, increasing to about 20% for ratios of 0.7, which is in the same range for mortars due to the admixture of aggregates. Long-term studies show reduced porosities and correspondingly reduced gas permeabilities over the 28-year test duration. For shotcrete, typically high w/c ratios imply porosities of 25 – 35%.

4.3.1 Gas-related characteristics of concrete

Water and gas permeabilities are different in concrete/mortar, where water is present in both the pore system and in the matrix as calcium silicate hydrate (CSH). Porewater flow may be affected by hydration or dissolution, depending on the chemical equilibrium of the fluid with concrete porewater. The typical range of intrinsic gas permeabilities for different concrete materials is given in Tab. 4-4.

Tab. 4-4: Typical ranges and suggested averages of concrete porosity and intrinsic permeability to water and gas

(From Nagra 2008).

Material	Porosity [%]	Intrinsic water permeability [m ²]	Intrinsic gas permeability [m ²]
High-performance concrete and waste packages	15%	10 ⁻¹⁹	10 ⁻¹⁷
Normal building concrete	20%	10 ⁻¹⁸	10 ⁻¹⁶
Shotcrete	25 – 35%	10 ⁻¹⁷	10 ⁻¹⁶
Average	25%	10 ⁻¹⁸	10 ⁻¹⁶

Gas permeability increases with the w/c ratio in concretes, and relative gas permeability decreases exponentially with increasing water content (Lanyon & Rüedi 2008, Jacobs 1998, Abbas et al. 1999, Monlouis-Bonnaire et al. 2003). The increase of capillary pressure with decreasing saturation is quite similar for different cements with air-entry pressures of 5×10^6 Pa and a van Genuchten n of about 1.5 to 2.5 (Monlouis-Bonnaire et al. 2003, Baroghel-Bouny et al. 1999).

4.3.2 Gas-related characteristics of mortar

High-porosity mortars were especially designed to provide high porosity for gas storage and transport while still withstanding high axial stresses (Jacobs et al. 1994). The mono-grain mortar (M1) and the flowing mortar (M2) were tested both on laboratory and larger-scale engineering experiments for different levels of compaction. Additionally, M2-type mortar with a lower w/c ratio as used for waste fixation at the Beznau nuclear power plant was tested. The porosities of the different types of mortars are summarised in Tab. 4-5 below. For experiments with M1 mortars, the results of small-scale and larger-scale tests were quite similar. The emplacement experiment of M1 mortar showed that, realistically, a density of up to about 1,800 kg/m³ can be reached. For M2 mortar, the emplacement experiment only reached densities of up to 1,900 kg/m³, with corresponding permeabilities between 10⁻¹³ and 10⁻¹² m². For mortars, experimental evidence indicates gas flow starts below 80% saturation, reaching a maximum around 30%. Water permeabilities start above 40 – 55% saturation, approaching the maximum permeability linearly (Jacobs et al. 1994). However, the range in capillary pressure measurements were only available to pressures up to 3,000 Pa, and available data were not consistent between mortars M1 and M2. The parameters resulting from modelling led to air-entry pressures of 500 Pa and a van Genuchten n of 2 (Mayer et al. 1999).

Tab. 4-5: Summary of results from small- and large-scale experiments with mortars M1 and M2

(From Nagra 2008).

Material	Density [kg/m ³]	Strength [N/mm ²]	Porosity [%]	Intrinsic water permeability [m ²]	Intrinsic gas permeability [m ²]
Mortar M1 (non-compacted)	1,650 ± 50	5.4	35 ± 3	¹ 3.1 ± 0.4 × 10 ⁻¹⁰	
Mortar M1 (compacted)	1,800 ± 50	10 ± 5	22 ± 3	¹ 2.7 ± 0.4 × 10 ⁻¹⁰ ² 4.4 ± 0.7 × 10 ⁻¹⁰	² 2.25 ± 0.3 × 10 ⁻¹⁰
Mortar M1 (highly compacted)	2,200 ± 50	34.6	23 ± 2	¹ 2.7 ± 0.4 × 10 ⁻¹⁰ ² 4.4 ± 0.7 × 10 ⁻¹⁰	² 2.25 ± 0.3 × 10 ⁻¹⁰
Mortar M2 (non-compacted)	¹ 2,200 ± 50 ² 1,450 ± 130 ³ 1,800	³ 15 ± 5	¹ 38 ± 2 ² 44 ± 10 ³ 32 ± 3	¹ 3.1 ± 0.6 × 10 ⁻¹⁴ ² 8 ± 5 × 10 ⁻¹² ³ 5 ± 4 × 10 ⁻¹³	
Mortar M2 (Beznau)	2,250		¹ 24 ± 2	¹ 2.5 ± 0.6 × 10 ⁻¹⁵	
Backfill	1,800		35	3 × 10 ⁻¹⁰	2.5 × 10 ⁻¹⁰

¹ Large-scale experiment (Mayer & Wittmann 1996; internal ref. in Lanyon & Rüedi 2008).

² Small-scale experiment (Jacobs et al. 1994).

³ Emplacement experiment (Mayer & Wittmann 1996; internal ref. in Lanyon & Rüedi 2008).

In order to cover the potential range in hydraulic and two-phase properties, an averaging process was performed based on the information of the different types of cements and mortars. The homogenisation of all cementitious materials in the backfill tunnel, described in detail in Nagra (2008), was derived as follows: porosities were averaged based on volumetric proportions, considering a range of values. Effective intrinsic permeabilities and relative gas permeabilities follow exponential decreases with increasing water saturation. Data consistency varies for different materials, and an approach based on the van Genuchten method is used to obtain average parameters linking pore-size distribution and capillary pressure.

4.3.3 Evidence from additional cement mixtures

As part of the data package by Flach et al. (2016), available information was compiled from existing studies on cementitious materials considered representative of cement mixes that could be used for encapsulation and/or solidification of waste for the Integrated Disposal Facility at the Hanford site in Washington State, USA. The information was provided in a form that considers uncertainty due to measurement error, variability from multiple samples using a given mix, and differences in properties associated with different mixes.

Values for saturated hydraulic conductivity (K_s), porosity (n), and dry bulk density (ρ_b) were compiled from various reports on cementitious waste forms and barriers. The data cover 21 mixes with various dry components blended with water or concentrated salt solution. The K_s values show a wide range and order statistics, a non-parametric analysis method (z-score), was used to analyse the dataset.

The log-probability plots were divided into three groups based on the dry materials having the greatest effect on hydraulic conductivity and contaminant mobility (Fig. 4-18):

- mixes with slag but neither sand nor aggregate;
- mixes with slag and sand and/or aggregate;
- mixes without slag but with sand and/or aggregate.

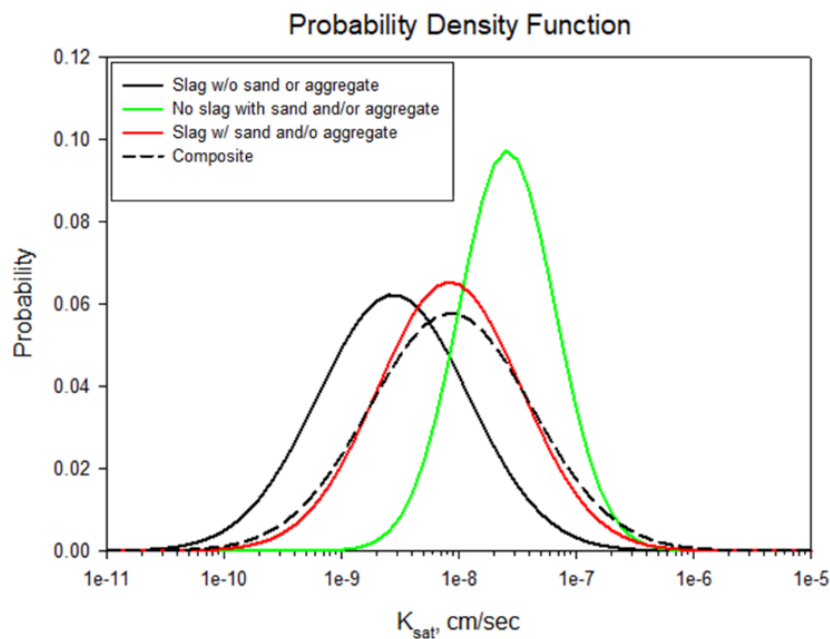


Fig. 4-18: Probability density functions for K_s in each subgroup and the overall population (Modified from Flach et al. 2016).

Summary statistics of $\log_{10}(K_s)$ for the groups and entire population are listed in Tab. 4-6. The best-estimate values for saturated hydraulic conductivity in Tab. 4-6 represent the geometric mean of the individual K_s values and the confidence interval as: $K_s^{BE} = 10^{\text{mean}[\log_{10}(K_{s,i})]}$. Summary statistics for dry bulk density (ρ_b) and water-exchangeable porosity (n) were calculated assuming normal distributions (Tab. 4-6).

Tab. 4-6: Summary statistics for K_s , dry bulk density, water-exchangeable porosity
(From Flach et al. 2016).

Statistic	w/ slag, w/o sand	w/o slag, w/ sand	w/ slag, w/ sand	All
Log10 [saturated hydraulic conductivity (cm/s)]				
Count (N)	39	31	19	98
Mean	-8.56	-7.59	-8.08	-8.07
Standard deviation (s)	0.64	0.41	0.59	0.68
Correlation coefficient (r^2)	0.97	0.97	0.87	0.97
Standard deviation of mean (s_m)	0.21	0.15	0.29	0.14
Saturated hydraulic conductivity (cm/s)				
Sample mean upper range ($+2s_m$); K_s^{PE}	4.5E-09	3.6E-08	1.6E-08	1.2E-08
Sample mean; K_s^{BE}	2.8E-09	2.6E-08	8.3E-09	8.5E-09
Sample mean lower range ($-2s_m$); K_s^{OE}	1.7E-09	1.8E-08	4.3E-09	6.2E-09
Dry bulk density (g/cm ³)				
Count (N)	39	31	18	97
Mean	1.07	1.98	1.88	1.59
Standard deviation (s)	0.13	0.08	0.07	0.44
Sample mean upper range ($+2s_m$)	1.12	2.01	1.91	1.68
Sample mean lower range ($-2s_m$)	1.03	1.95	1.84	1.50
Porosity (cm ³ void/cm ³ total)				
Count (N)	28	31	18	86
Mean	0.59	0.18	0.24	0.33
Standard deviation (s)	0.03	0.05	0.03	0.19
Sample mean upper range ($+2s_m$)	0.60	0.20	0.25	0.37
Sample mean lower range ($-2s_m$)	0.58	0.17	0.22	0.29
Solid density (g/cm ³) ¹				
Count (N)	29	31	18	86
Mean	2.47	2.43	2.46	2.45
Standard deviation (s)	0.11	0.07	0.06	0.08
Sample mean upper range ($+2s_m$)	2.68	2.54	2.53	2.62
Sample mean lower range ($-2s_m$)	2.32	2.27	2.27	2.27

Moisture-retention properties of samples were determined using laboratory measurements of pressure head and moisture content. Curve fitting is used to estimate the parameters in the van Genuchten model defining the moisture retention curves, shown in Fig. 4-19.

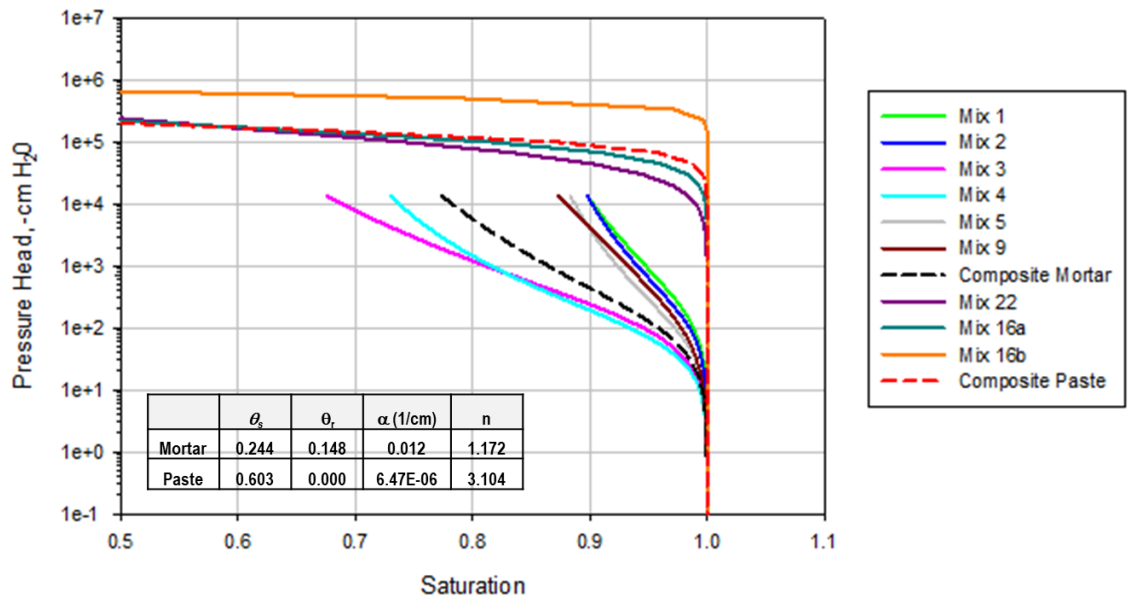


Fig. 4-19: Fitted van Genuchten parameters for different mixes and averaged values for mortar and paste

(From Flach et al. 2016).

The van Genuchten (1980) parameters for mortar and paste imply a unimodal moisture characteristic curve and are not capable of matching water-retention data from bimodal samples (e.g., Zurmühl & Durner 1998). However, a linear superposition of two van Genuchten functions can represent the combined effect of two distinct subpopulations of pore sizes (e.g., Durner 1994). Flach et al. (2016) developed bimodal curves, where the total mortar porosity is composed of a contribution from cemented sand/aggregate and pure paste fraction, which could be applied to any specific grout formulation that contains various amounts of cement, fly-ash and slag, or a sand/aggregate mortar.

4.3.4 Reference parameters of L/ILW Nearfield Materials

Emplaced near-field materials used in the L/ILW repository include the M1 mortar, LC-86H container, waste package, container filling (Dorodur), liner, support concrete and cavern sole. The corresponding hydraulic and two-phase flow parameters are summarised in Tab. 4-7.

Tab. 4-7: Hydraulic and two-phase properties for the L/ILW near-field materials

	Symbol, unit	M1 mortar	LC-86H container	Waste package, Dorodur	Liner, concrete
Hydraulic parameters					
Porosity	ϕ [-]	0.20	0.10 ^b	0.35	0.10 ^b
Intrinsic permeability	k [m ²]	1.E-10	3.E-16	1.E-15	3.E-16
Pore com-pressibility	C_p [1/Pa]	3.0E-10	5.0E-10	5.0E-10	7.0E-10
Initial water content	w_r [%]	12.	5.0	25.	7.0
Initial saturation ^c	S_w [-]	0.50	0.33	0.70	0.70
Two-phase flow parameters					
van Genuchten capillary strength ^a	P_0 [Pa]	5.E02	2.E06	1.E06	2.E06
Shape para-meter	vG-n (k_r) vG-n (P_c)	2.0	2.0	2.0	2.0
Residual water sat.	$S_{lr}(kr)$	0.05	0.05	0.05	0.05
	$S_{lr}(Pc)$	0.01	0.01	0.01	0.01
Residual gas saturation	$S_{gr}(kr)$	0.0	0.0	0.0	0.0

^a Default value $T_0 = 20$ °C for temperature scaling.

^b Total porosity: 12 – 14%, capillary pores 7 – 8%.

^c Varied in assessment cases.

5 Summary and conclusions

This report summarises and integrates the lines of evidence which have proven beneficial for broadening the existing gas-related database of the host rock (Opalinus Clay) and the confining geological units in the three potential siting regions for a deep geological repository in Northern Switzerland. Gas-related properties and THM properties of the geological barriers and the engineered barrier system (EBS), such as porosity, intrinsic permeability, relative permeability, capillary pressure, thermal conductivity and heat capacity provide an input for model-based assessments of repository-induced effects in the context of the site selection process and for the PA/SA-related modelling of gas release, contributing to the safety case for a combined repository in the NL siting region.

The report provides a brief introduction to the fundamentals of gas transport in porous media. A comprehensive survey of the available field and laboratory data is compiled and documented. Data sources include previous site investigation programmes, the latest deep borehole campaign conducted in the three potential siting regions, RD&D activities at the Mont Terri URL and on other international research platforms (including the EURATOM projects NF-PRO, FORGE, EURAD-GAS). The gas-related databases are interpreted and subjected to model-supported analyses, finally constituting the gas-related reference dataset for the Opalinus Clay, for the confining geological units in the three siting regions and for the EBS.

5.1 Phenomenology of gas transport in the proposed host rock formations

Gas release paths through the host rock

The phenomenological description of flow and transport processes in porous media is closely tied to their fabric and the inventory of textural and structural features. In claystone formations such as the Opalinus Clay and the clay-rich sequences of the confining geological units with clay contents > 40%, the swelling capacity of the rock ensures that brittle features (fractures) are tight, when burial depth exceeds several decametres. Thus, flow and transport processes are restricted to intrinsic porosity of the rock matrix (as long as pore pressure is significantly below lithostatic pressure; see also next section on gas transport mechanisms). Essentially, a network of connected pores in the range of micro- to nanometres defines the space where flow of immiscible fluids can occur. As a consequence, gas transport processes in claystones are controlled by the spatial variability of their mineralogical and petrophysical properties. Laboratory investigations on undisturbed rock samples can provide reliable estimates of gas-related properties.

In fractured, low-porosity rocks such as the calcareous sequences of the confining geological units in the NL siting region, gas transport processes are limited to the more permeable fracture systems, whereas the rock matrix is essentially impermeable to gas (relative to the much larger gas flow rates in the fracture systems). Consequently, gas transport in fractured rock is essentially controlled by site-specific characteristics such as the density and connectivity of the fracture systems, the prevailing tectonic regime, in-situ stress and pore-pressure conditions rather than by the intrinsic rock properties. Laboratory investigations on undisturbed rock samples may not be representative for the effective gas transport parameters on the repository scale; instead, they provide a lower bound for the gas transport capacity of the rock.

Gas transport mechanisms

Advection and diffusion of dissolved species represent the simplest transport mechanisms in a water-saturated porous medium. The propagation of the dissolved species is controlled by the water velocity and its extent is controlled by the hydrodynamic dispersion – a well-known aggregate representation of the mixing processes due to diffusion, Taylor dispersion and tortuosity. The dissolution of a gaseous species in water is described by Henry's law, the diffusion of the dissolved gas is represented by Fick's law and the viscous losses of the porewater flow in the pore network are expressed by Darcy's law. Advection, diffusion and dissolution are well-established transport and retention mechanisms and corresponding parameter sets (intrinsic permeability, effective diffusion coefficients, solubility) with the corresponding uncertainty ranges have been elaborated for all host rock formations.

Two-phase flow conditions occur when gas invades a water-saturated porous medium in a separate phase. The propagation of the gas front is controlled by the interaction of gravity, viscous forces and capillary forces. In fluid mechanics, flow of immiscible fluids is often described in terms of dimensionless numbers, namely the capillary number, the mobility ratio and – if gravity plays a role – the Bond number. Thus, scale dependence of the transport processes can be expressed in a universal way by introducing dimensionless length scales, which allows the transfer of the basic flow laws to other scales of interest. Broad experimental evidence has been established in experimental fluid mechanics with regard to the analysis and classification of immiscible fluid flow processes in porous media. Within the classification schemes of fluid mechanics, gas transport processes in claystones and shales are characterised by very low capillary numbers and can thus be assigned to the flow regime of capillary fingering. Capillary fingering is associated with instable displacement of the wetting fluid (water) by the non-wetting fluid (gas), giving rise to phenomena such as migration, fragmentation and coalescence of the non-wetting fluid. The basic principles of two-phase flow and the corresponding equations of motion (water, gas) are well-established as well as the associated parametric models for the capillary pressure-saturation relationship and relative permeability. Reference values for the two-phase flow parameters (i.e., capillary strength/gas entry pressure, pore-size factor, residual water/gas saturation) have been elaborated for all host rock formations together with the corresponding uncertainty ranges.

The degree of complexity increases, when two-phase flow processes occur in a deformable porous medium. Porosity is no longer an intrinsic characteristic of the porous medium but depends on the total stress and the applied gas pressures. Thus the state of deformation, the porosity evolution and the corresponding change in permeability are defined by the actual stress path acting on the porous medium. From a phenomenological point of view, gas transport in deformable porous media can be divided into two regimes, namely dilatancy-controlled gas flow ("pathway dilation") and gas fracturing.

Pathway dilation is associated with ductile fracturing. Gas-driven microfracturing leads to an increase in porosity, which is accompanied by a detectable increase in intrinsic permeability and a change in the capillary pressure-saturation relationship. In the terminology of multiphase-flow concepts, gas flow is yet controlled by visco-capillary forces. The main difference with respect to conventional two-phase flow is that the transport properties of the solid phase (rock permeability, relative permeability, capillary pressure relationship) can no longer be viewed as invariants since they depend on the state of deformation of the rock. Theoretical frameworks have been established in the fields of fracture mechanics and material research to conceptualise and model ductile fracturing in porous media. However, the application of such concepts on gas transport in shales and claystones is a subject of ongoing research. For simple stress paths, pragmatic solutions have been proposed in reservoir engineering literature, representing the functional relationship between

deformation and permeability by pressure-dependent permeability multipliers. The permeability multiplier approach has been adopted for modelling gas release in the geosphere when gas pressure exceeds the threshold pressure for pathway dilation.

Gas fracturing is associated with the creation of brittle fractures. A brittle fracture is initiated quasi-instantaneously without precursory plastic deformation and propagates at about the velocity of a shear wave. Gas flow in such a macroscopic tensile fracture can be seen as a single-phase flow process. In a rock with low tensile strength (e.g., claystones), a macroscopic fracture develops only when the gas pressure build-up is rapid, i.e., when the combined effect of porewater displacement and formation of small-scale fractures (i.e., dilatancy) no longer counterbalances the gas production rate. The conceptual, theoretical and experimental framework for fracture propagation is well documented in standard reservoir engineering literature.

5.2 Reference parameters of the host rock formation and confining geological units

A comprehensive set of geotechnical rock properties and constitutive relationships is needed for modelling gas-transport processes in the host rock formations, comprising total porosity, intrinsic permeability, capillary pressure and relative permeability. In the clay-rich host rock formations with typical clay contents > 40% (Opalinus Clay, clay-rich sequences of the confining geological units), representative property estimates can be derived from laboratory tests on core samples. For those confining geological units with low and moderate clay-content, laboratory tests on core samples can provide lower bounds for their gas transport capacity; complementary site-specific knowledge is required concerning the hydraulic significance of the fracture systems to derive representative estimates of their effective gas transport properties.

In the context of Stage 3 of the SGT, the experimental database on gas-related properties has been considerably expanded, particularly addressing the water-retention behaviour and relative permeability / water-saturation relationship of the Opalinus Clay. Advanced water-/gas-permeability test set-ups were developed, providing new insight into the hydro-mechanical coupled processes associated with transport and providing high quality datasets for benchmarking two-phase flow modelling approaches.

Opalinus Clay

Hydraulic parameters and two-phase flow parameters (“gas-related properties”) of the Opalinus Clay exhibit a depth dependence of porosity, permeability and capillary strength. The reference values of gas-related properties of the undisturbed Opalinus Clay presented in Tab. 3-5 refer to repository conditions with a typical overburden of more than 500 m, indicating hydraulic conductivities which are about 1 – 2 orders of magnitude lower than the values at Mont Terri. The reference parameters and the corresponding uncertainty ranges (“alternative values”) are well-supported by the latest experimental database from the TBO site investigation programme conducted within the framework of Stage 3 of the SGT (Nagra 2024a).

Clay-rich sequences of the upper confining geological units

A set of reference parameters has been elaborated for the clay-rich sequences of the upper confining units (formerly called «Brauner Dogger»), drawing mainly on laboratory tests with core samples from the clay-rich sequences in the Schlattigen SLA-1 borehole. As expected, the derived two-phase flow properties are similar to those from the deep Opalinus Clay. The reference values and the corresponding uncertainty ranges (“alternative values”) for the «Brauner Dogger» are given in Tab. 3-8.

Calcareous and sandy sequences of the confining geological units

Gas transport in the calcareous and sandy sequences of the «Effingen Member», a potential host rock formation of the former Jura-Südfuss siting region was characterised as part of the site investigation programme in Stage 2 of the SGT (Senger et al. 2014a). The investigations revealed that gas transport in the calcareous and sandy sequences is not only controlled by the spatial variability of intrinsic permeability of the sedimentary structures, but also by the occurrence of brittle tectonic features and their site-specific characteristics. High interval transmissivities in packer tests are linked exclusively to test intervals in the calcareous sequences, suggesting that fracture flow dominates in those lithologies. In the calcareous marls, the interval transmissivities are generally low, which is regarded as a strong indication for matrix flow.

Thus, different sets of reference parameters were specified for the calcareous marl sequences (KMA), the limestone bed sequences (KBA), and the Gerstenhübel Beds (GER), based on the derived average hydraulic conductivities of the different sequences, which are summarised in Tab. 3-9. In terms of two-phase flow parameters, the WRC data are representative of the low-permeability KMA sequence, whereas the capillary-strength parameter is scaled to lower values for the higher permeable KBA and GER sequences.

According to the acquired structural databases from the Jura-Südfuss siting region, the role of the fracture systems depends significantly on the local conditions. The high spatial variability of the fracture frequency with a distinct clustering suggests a high variability in the gas transport capacity of the fracture systems in the Effingen Member.

The lower clay content of the sandy-calcareous sequences (SKA) gives rise to an enhanced permeability, which is evidenced by in-situ packer testing. No distinction between KMA and SKA is made with regard to the capillary strength and the pore-size factor due to the lack of site-specific experimental evidence. In this context, the comparison with evidence from additional, externally obtained evidence (Mesaverde gas shales, Rotliegendes sandstones; see Section 3.4) suggests a decrease of capillary strength with increasing permeability, implying that the capillary strength of the SKA could be slightly overestimated.

5.3 Gas transport in the proposed EBS materials

MX-80 Bentonite

Extensive research and technology development surrounding the use of bentonite clay and mixtures as buffers, seals, or backfills have been conducted in geological disposal programs (Sellin & Leupin 2013). Early experiments by Pusch and colleagues on various bentonite types examined gas transport behavior, noting a linear relationship between gas flow rate and pressure gradient in unsaturated or partially saturated bentonite. Subsequent studies by Pusch & Forsberg (1983) on MX-80 bentonite identified a critical gas breakthrough pressure related to the swelling pressure of the clay. Further experiments on MX-80 by Horseman et al. (1997) emphasised the importance of swelling pressure on gas transport for initially saturated bentonite, with gas breakthrough occurring just above the swelling pressure. Harrington & Horseman (1999) suggested that effective gas permeability depends on pressure-induced pathways rather than being an inherent material property. Sellin (2014) reported local gas injection experiments showing the formation of dilatant pathways in bentonite above critical pressures, with unstable flow and no measurable desaturation. Graham et al. (2016) also showed the link between the gas pressure at which entry is observed and total stress, whereby the breakthrough pressure is significantly higher than the gas entry pressure for stress states representative of expected repository conditions.

Gas injection tests in fully water-saturated samples of compacted granular MX-80 bentonite (Fig. 4-8), reported in Romero & Gonzalez-Blanco (2019), indicated during the constant-rate gas injection phase sample expansion with only very small outflow detected. After shut-off, the sample expansion continued because of the gas pressure front propagation into the sample. Axial deformation reversed as the outflow rate started to drastically increase and the injection pressure started to decrease, which induced sample compression as the constitutive stress increased (Fig. 4-8). The corresponding μ -CT images (Fig. 4-3) showing the distribution of macro-pores associated with the compaction, saturation, and post gas injection states indicate the well-connected intergranular porosity after compaction; after saturation, many of the large pore channels disappear due to swelling, which is compensated by the increase of meso- and micro-porosity. After gas injection, the μ -CT images show a network of distinct pore channels along the grain boundaries similar to that from the compacted stage, which was confirmed by the grain-size distribution analyses by Keller (2019) in Romero & Gonzalez-Blanco (2019).

As part of Task 7 of the EBS Task Force different modeling concepts were developed to simulate the gas injection test accounting for the injection pressure and outflow response as well as the measured axial strain of the core sample using two-phase coupled HM or two-phase models with a simplified HM coupling (Section 4.1.2), which are too complex for the repository-scale modeling. For the PA/SA-related modeling of gas release from geological repositories in the candidate siting region the relevant input parameters for the different bentonite materials are summarised in Tab. 4-2.

Sand / Bentonite

In the Swiss deep geological disposal concept, S/B mixtures with low bentonite content (20 – 30%) are considered suitable sealing and backfilling materials for underground structures, forming the “engineered gas transport system” (EGTS) of the L/ILW repository. The EGTS aims to improve gas transport in underground structures without compromising radionuclide retention. S/B mixtures increases gas transport capacity without significantly increasing water permeability or reducing swelling pressure, and the addition of sand enhances mechanical stability and thermal conductivity.

The geotechnical characteristics and water retention of S/B mixtures is largely based on work by Manca (2016), summarised in Section 4.2, using granular S/B mixtures compacted to dry densities of 1.50 and 1.80 g/cm³. Index testing examined the dependence of index properties on water composition. Liquid limit decreases with increasing osmotic suction of water used for testing, while the plastic limit is only slightly affected by water composition. Higher pore water salinity reduces the mixture’s activity, indicating a reduction in the swelling capacity of the bentonite fraction due to the lower swelling capacity of smectite minerals at the particle level. The presence of sand grains in the mixture contributes to the relatively low liquid and plastic limits compared to pure bentonite.

Water retention behavior of these mixtures for total suctions above 3 MPa, was found to be relatively consistent for both compaction densities, suggesting that compaction density has a minimal effect on water retention. The measured relative permeability curves displayed hysteresis for both dry densities. Hysteresis was observed in the hydraulic conductivity versus suction curve, which was associated with irreversible deformation of the internal structure of bentonite during wetting and drying cycles, indicating that S/B mixtures allow gas passage at lower pressures while still limit pore water flow. For the PA/SA-related modeling the relevant input parameters for the different S/B mixture are given in Tab. 4-3.

Concrete / Mortar

Normal concretes and mortars will be used for engineering purposes as well as for waste packaging. The primary requirements of these materials is their static behaviour and the ability to retain water inflow into the tunnel during construction and emplacement. High porosity mortars were designed to provide high porosity for gas storage and transport as well as withstanding high axial stresses.

Relevant information on concrete and mortar was based largely on experiments performed at ETH summarised in Tab. 4-4 and Tab. 4-5 in Section 4.3, by Mayer et al. (1992), Mayer & Wittmann (1996), Mayer et al. (1999) and recent French studies, which was compiled in Appendix A of Nagra (2008).

For the PA/SA-related modeling, the relevant input parameters for the different concrete and mortar materials are given in Tab. 4-7.

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