Hydro-mechanical response of Opalinus Clay in the CO₂ long-term periodic injection experiment (CO₂LPIE) at the Mont Terri rock laboratory

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Abstract Guaranteeing the sealing capacity of caprocks becomes paramount as CO₂ storage scales up to the gigaton scale. A significant number of laboratory experiments have been performed with samples of intact rock, showing that low-permeability and high-entry pressure caprocks have excellent sealing capacities to contain CO₂ deep underground. However, discontinuities, such as bedding planes, fractures and faults, affect the rock properties at the field scale, being at the same time challenging to monitor in industrial-scale applications. To bridge these two spatial scales, Underground Research Laboratories (URLs) provide a perfect setting to investigate the field-scale sealing capacity of caprocks under a well-monitored environment. In particular, the CO₂ Long-term Periodic Injection Experiment (CO₂LPIE) at the Mont Terri rock laboratory, Switzerland, aims at quantifying the advance of CO₂ in Opalinus Clay, an anisotropic clay-rich rock with bedding planes dipping 45° at the experiment location. To assist in the design of CO₂LPIE and have an initial estimate of the system response, we perform plane-strain coupled Hydro-Mechanical simulations using a linear transversely isotropic poroelastic model of periodic CO₂ injection for 20 years. Simulation results show that pore pressure changes and the resulting stress variations are controlled by the anisotropic behavior of the material, producing a preferential advance along the bedding planes. CO₂ cannot penetrate into Opalinus Clay due to the strong capillary effects in the nanoscale pores, but advances dissolved into the resident brine. We find that the pore pressure oscillations imposed at the injection well are attenuated within tens of cm, requiring a close location of the

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monitoring boreholes with respect to the injection interval to observe the periodic signal.

**Article highlights**

- Underground rock laboratory experiments permit examining the caprock sealing capacity at a representative scale for CO₂ storage;
- We perform coupled transverse isotropic hydro-mechanical simulations to gain insight on the response of shaly rock to CO₂ periodic injection;
- Simulation results assist in the design of the injection amplitude and period and monitoring of the long-term periodic CO₂ injection experiment.

**Keywords**  Geologic carbon storage · Geomechanics · Caprock integrity · Shale · Transverse isotropy

1 Introduction

Effective scenarios to mitigate climate change should target rapid global decarbonization and net withdrawal of CO₂ from the atmosphere (IPCC 2014; Warszawski et al. 2021). A feasible and credible solution to substantially reducing anthropogenic CO₂ emissions and achieving carbon neutrality is Carbon Capture and Storage (CCS) in geological formations at the gigaton scale (Bui et al. 2018; Ringrose et al. 2021). The best-practice guidelines suggest injecting CO₂ at depths greater than 800 m to ensure that it stays in the supercritical state (IEA GHG 2009; Miocic et al. 2016). Relatively high density of supercritical CO₂ increases the subsurface storage capacity and alleviates buoyancy forces driving upward migration of CO₂ (Bachu 2003). However, CO₂ is still buoyant at temperature (>31 °C) and pressure (>7.38 MPa) conditions of sedimentary basins considered for CCS, raising concerns about potential leakage to shallow groundwater aquifers or even back to the surface and into the atmosphere. As a result, large-scale deployment of CCS and long-term CO₂ containment in the subsurface relies primarily on competent caprock formations hindering upward CO₂ migration out of the reservoir complex.

Over three decades of research and practice in geologic carbon storage provide invaluable insights into the Hydro-Mechanical (HM) behavior of the caprock controlling the long-term fate of injected CO₂. Much can be learned from laboratory experiments, numerical simulations, and monitoring of CO₂ storage sites or naturally occurring reservoirs. Breakthrough experiments have provided a reliable measure of capillary properties for intact caprock samples under representative subsurface conditions (Hildenbrand et al. 2002; Boulin et al. 2013; Makhnenko et al. 2017; Minardi et al. 2021). These experiments render high capillary entry pressures in the order of several MPa for shaly caprocks, making these formations appropriate to act as a seal for CO₂ storage. However, injection-induced overpressure and potential CO₂ intrusion into the caprock may lead to pore system expansion and caprock damage that could potentially deteriorate the caprock sealing capacity (Rutqvist 2012; Vilarrasa et al. 2015). In particular, the pressure-induced expansion of the lowermost portion of the caprock at the In Salah storage site had a significant contribution to the measured surface uplift (Rutqvist et al. 2010). More importantly, expansion causes an increase in porosity, which may significantly enhance permeability even for small porosity increments because the permeability–porosity relationship for caprock can take a power-law form with exponents in the range of 15 to 17 (Kim and Makhnenko 2020). At the same time, simulation results of lab- and field-scale CO₂ injections indicate that CO₂ may penetrate into the caprock in the range from a few centimeters to meters (Rutqvist et al. 2008; Vilarrasa et al. 2010a; Kivi et al. 2022).

Laboratory experiments on centimeter-scale caprock specimens provide key insights into relevant HM processes and are necessary for initializing numerical simulations, but can hardly deal with field-scale complexities. Heterogeneities on varying scales, starting from pores and microfractures to bedding planes and fault zones that are several meters thick, can be present in the caprock and may provide preferential flow paths as well as localized deformations (Rutqvist and Tsang 2002; Rutqvist et al. 2016). For example, the fast vertical migration of the CO₂ plume across the thin mudstone layers in the Sleipner storage site is analyzed to be indicative of pervasive fracturing with effective capillary entry pressures 35 times smaller than those measured in the laboratory on intact shale specimens (Cavanagh and Haszeldine 2014). Plausible alterations of the rock microstructure and water content over the course of coring and sample
preservations, as well as the inability to reproduce the subsurface temperature and stresses in the laboratory, raise questions about the full representativeness of the laboratory experiments and inferred conclusions (Vilarrasa et al. 2017). Therefore, growing efforts are devoted to developing and exploiting precise techniques of monitoring CO₂ injection projects. Previous monitoring efforts primarily targeted the CO₂ plume migration (Arts et al. 2003), pressure changes in the overlying aquifers (Kim and Hosseini 2014), induced seismicity (Verdon et al. 2011) and surface uplift (Ringrose et al. 2013) to demonstrate secure storage of CO₂ with minimum detrimental environmental impacts.

Field-scale CO₂ injection poses challenges in monitoring at increasing depths, as well as in the interpretation of the ongoing processes. To address these challenges, controlled underground rock-laboratory experiments at meter to decameter scale have drawn special attention to fill the gap between the core scale (cm) and industrial-scale (km) observations (Bossart et al. 2017a). These experiments take advantage of realistic conditions of the subsurface, thoroughly characterized geological settings, controlled injection conditions, and detailed and comprehensive monitoring in the proximity of the injection zone. The meso-scale experiments can be useful to bring the knowledge of CO₂ leakage mechanisms into maturity.

**Fig. 1** Schematic representation of the geological setting and location of the CO₂LPIE experiment (CL niche) at the Mont Terri rock laboratory. The new tunnels and niches are highlighted in green
improve simulation models, develop and examine innovative monitoring approaches, and establish strategies and protocols to ensure long-term caprock integrity.

The CO₂ Long-term Periodic Injection Experiment (CO₂LPIE) aims at investigating the sealing capacity of a caprock in response to direct CO₂ injection at the decameter scale (Rebscher et al. 2020). CO₂LPIE will be carried out in a highly monitored environment in the Mont Terri Underground rock laboratory, Switzerland (Fig. 1). The host rock for CO₂LPIE is Opalinus Clay, a claystone with high capillary entry pressure and low permeability, considered to be a good representative caprock for CO₂ storage (Bossart et al. 2017a; Vilarrasa and Makhnenko 2017; Minardi et al. 2021; Zappone et al. 2021). At an appropriate distance from the injection point, observation boreholes will be drilled and instrumented with high-resolution pressure transducers and deformation sensors. This setting allows continuous monitoring of pressure changes and rock deformation, as well as geochemical sampling while recording the injection flow rate and fluid pressure. Given the low intrinsic permeability of the shale, optimizing the injection scheme and accurately locating the monitoring boreholes become a priority. An effective recording of the rock response should be guaranteed, while obeying the constraints given by (a) the extension of the zone disturbed by the drilling process and (b) the need to prevent a hydraulic connection between boreholes.

The main objective of this study is to assist in designing CO₂LPIE in the light of preliminary numerical modeling of the involved HM processes. We first present a brief description of the Mont Terri rock laboratory, the geological structures, and the CO₂LPIE experimental setting. We then focus on 2D fully coupled HM numerical simulations. In addition, we describe the relevant governing equations, the model geometry, initial and boundary conditions, and material properties. Next, we describe the performed sensitivity analyses, including variations of the amplitude of the periodic injection and rock properties. Here, results on the pore pressure development and stress perturbations due to CO₂ injection in different scenarios are of special interest. Finally, we discuss the inferred HM behavior and how it helps with the design of the CO₂ injection scheme and the monitoring program.

2 Overview of the Mont Terri rock laboratory and the CO₂LPIE experiment

The Mont Terri rock laboratory is located near St. Ursanne, in the North-West of Switzerland, and is operated by the Swiss Federal Office of Topography, swisstopo. The rock laboratory is nested at approximately 280 m below the Earth’s surface and is accessible through the safety gallery of a nearby motorway tunnel, passing through the Jura Mountains (Fig. 1). It has experienced a quarter-century period of development and constitutes an international and unified platform for cutting-edge research in the field of underground storage and waste disposal (see Bossart et al. 2017a for a review). The rock laboratory is excavated in the Aalenian-Toarcian age Opalinus Clay, deposited around 174 million years ago (Nussbaum et al. 2011). Owing to its ultralow permeability, Opalinus Clay has been primarily investigated as a potential repository host rock for nuclear waste and, more recently, as a representative caprock for geologic CO₂ storage. In this context, a variety of experiments were performed, concentrating, for example, on Thermo-Hydro-Mechanical (THM) behavior of Opalinus Clay (HE, Heating Experiment, Bossart et al. 2017b), seasonally-induced HM processes (CD, Cyclic Deformation experiment, Ziefle et al. 2017), diffusion and sorption processes (DI, In Situ Diffusion, DR, Diffusion and Retention, and FM-C, Flow Mechanism experiments, Leupin et al. 2018), the CO₂ sealing capacity of a clayey fault (CS-D, Carbon Storage experiment, Zappone et al. 2021) and fluid injection-induced earthquake rupture and fault reactivation (FS, Fault Slip experiments, Guglielmi et al. 2020).

The CO₂LPIE experiment plans to inject CO₂ in pristine Opalinus Clay at the Mont Terri rock laboratory in a long-term (> 10 years) periodic fashion. CO₂LPIE is targeted at exploring the following:

1. the effective hydraulic and mechanical properties of the seal at the rock mass scale;
2. the effect of the cyclic injection scheme on the transient pore pressure evolution and rock deformation;
3. the extent to which CO₂ can penetrate into the intact caprock;
4. the Hydro-Mechanical-Chemical (HMC) processes governing CO₂ intrusion into and transport through caprock; and
5 potential alterations of the rock hydraulic and mechanical behavior in response to pressurization and chemical fluid-rock interactions.

CO$_2$LPIE will be carried out in the CL niche, oriented perpendicular to the minimum horizontal stress direction and the new Gallery 18. Here, the bedding planes dip 45° towards the SSE. CO$_2$LPIE will be performed through an inclined injection borehole, drilled from the sidewall of the niche with a diameter of 0.086 m and a length of about 10 m perpendicular to the local bedding planes (Fig. 2). The plan is to inject CO$_2$ at a 0.2 m long segment at the lowermost portion of the borehole and far away from the excavation damage zone that extends to 1–2 m from the niche’s wall (Bossart et al. 2002). As a consequence, we assume that the host rock is intact and fully saturated having negligible pore pressure and stress perturbations. The stress regime is estimated to be normal faulting, meaning that the maximum principal stress $\sigma_1 \approx 6.5$ MPa is close to vertical and roughly conformed to the overburden weight. The intermediate and minimum principal stresses are sub-horizontal with the values of $\sigma_2 \approx 4.0$ MPa and $\sigma_3 \approx 2.2$ MPa, respectively (Martin and Lanyon 2003; Corkum 2006).

Multiparameter monitoring will be performed using high-resolution sensors installed in both the injection borehole and adjacent observation boreholes. Injection pressure and flow rate will be recorded together with the induced rock deformation, perturbed pore pressure, and geochemical parameters of interest. Rock samples will be retrieved for complementary laboratory investigations. The laboratory tests will allow understanding possible fluid-rock chemical interactions and their impacts on the hydraulic and mechanical properties of the rock, to develop and calibrate constitutive models, and to assist in more efficient interpretation of the recorded data. Nevertheless, the design phase of CO$_2$LPIE also reaps the benefits of interpretative modeling for the best adjustment of the injection parameters and the monitoring setup. The model inception task is integrated with preliminary laboratory measurements of rock properties, which will be addressed in this paper with a primary focus on the governing HM processes. The main advantages of such a multidisciplinary elucidation of the recorded data are: (1) more realistic treatment of the caprock with CO$_2$ injection,
advancing our knowledge of the underlying chemical and HM effects and (2) improved prediction capabilities of numerical models for field- and basin-scale CCS projects.

3 Methodology

3.1 Description of the hydro-mechanical model

We simulate the HM response of Opalinus Clay to CO₂ injection using the finite element code CODEBRIGHT (Olivella et al. 1994; 1996), which allows for solving a wide range of THM problems in porous media, including CO₂ storage in deep geological formations (Vilarrasa et al. 2010a). CO₂ injection into the brine-saturated rock induces a two-phase flow of brine and CO₂ as the wetting and non-wetting phases, respectively. Besides, CO₂ partially dissolves into water, initiating diffusive transport of dissolved CO₂ species in the brine phase. In order to simulate the coupled rock deformation and flow phenomena, the code simultaneously solves the mass conservation equation for the present components (here CO₂ and water) and the momentum balance. The mass balance equation for each component writes as

\[
\frac{\partial}{\partial t} \left( \omega_i \rho_i S_i \phi + \omega_s \rho_s S_s \phi \right) + \nabla \cdot \left( \dot{\mathbf{r}}_i + \mathbf{v}_i + \omega_i \rho_i \mathbf{q}_i + \omega_s \rho_s \mathbf{q}_s \right) = f^i, \ i = c, w
\]

(1)

where \( \omega_i \) is the mass fraction of component \( i \) (\( c \) for CO₂ and \( w \) for water) in each phase, and \( S_i \) is the saturation of \( i \) phase. Here, \( \psi \) can be either \( l \) or \( g \) for the liquid and gas phases, respectively. The second term on the left-hand side denotes the conceivable flow mechanisms involving advective phase flux \( \mathbf{q} \) and diffusive flux of individual components \( \dot{\mathbf{r}}_i \). The right-hand side \( f^i \) accounts for an external source or sink of component \( i \). The volumetric flow rate of the \( \psi \) phase is related to the existing pressure gradient and gravity, reading from Darcy’s law as

\[
\mathbf{q}_\psi = -\frac{k \mu_\psi}{\mu_\psi} (\nabla p_\psi + \rho_\psi g \nabla z), \ \psi = l, g
\]

(2)

where \( k[L^2] \) is the anisotropic intrinsic permeability tensor accounting for preferential flow paths along bedding planes, \( p_\psi[ML^{-1}T^{-2}] \) is the \( \psi \)-phase pressure, \( k_\psi[-] \) and \( \mu_\psi[ML^{-1}T^{-1}] \) represent the relative permeability and dynamic viscosity of the fluid phase \( \psi \), respectively, \( g[LT^{-2}] \) is the gravity acceleration, and \( z[L] \) is elevation.

The molecular diffusion of the dissolved species is governed by Fick’s law

\[
\dot{\mathbf{r}}_\psi = -\tau \phi \rho_\psi S_\psi D_\psi \nabla \phi_\psi
\]

(3)

where \( \tau \) expresses the pore network tortuosity and \( D_\psi[L^2T^{-1}] \) the diffusion coefficient of component \( i \) in phase \( \psi \). The product of tortuosity and diffusion coefficient represents the effective diffusion coefficient \( D \) of each component across the pore network. In our numerical simulations, we neglect diffusive transport of water vapor in the CO₂ phase, i.e., \( \dot{\mathbf{r}}_g = 0 \).

The numerical model satisfies the linear momentum balance for the porous medium, which writes as

\[
\nabla \cdot \mathbf{\sigma} + \mathbf{b} = 0
\]

(4)

where \( \mathbf{\sigma}[ML^{-1}T^{-2}] \) is the total stress tensor and \( \mathbf{b}[ML^{-2}T^{-2}] \) the vector of the body forces. The constitutive behavior of the porous rock is established using linear poroelasticity (Cheng 2016)

\[
\mathbf{\sigma} = C \epsilon + \alpha \mathbf{p}
\]

(5)

where \( \epsilon[-] \) is the strain tensor, and \( \mathbf{p}[ML^{-1}T^{-2}] \) is the pore pressure set as \( p = \max(p_l, p_g) \). The elastic modulus tensor \( C[ML^{-1}T^{-2}] \) defines the relation between effective stress \( \mathbf{\sigma} = \mathbf{\sigma} - \alpha \mathbf{p} \) and the strain tensor. \( \alpha[-] \) represents the Biot effective stress coefficient tensor, assumed to be isotropic (\( \alpha = a \mathbf{I} \)), with a value of scalar \( a \), and \( \mathbf{I} \) the identity tensor. Following the transversely isotropic model defined by Cheng (1997), the elastic tensor is assumed to replicate the mechanical behavior of the host rock with bedding planes. Therefore, five elastic moduli are required to define the material model. Considering the generic plane \( x'z' \) aligned parallel to the bedding planes and \( y' \)-direction perpendicular to them (see Fig. 3), the elasticity tensor entries are expressed by the Young’s moduli \( E_{x'} = E_{y'} = E_p \), \( E_{z'} = E_n \), the Poisson’s ratios \( \nu_{x'} = \nu_{y'} = \nu_p \), \( \nu_{z'} = \nu_n \), and the shear modulus \( G_{x'} = G_{y'} = G_n \), where the subscripts \( p \) and \( n \) imply the directions parallel and normal to the bedding planes,

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respectively. Accordingly, the behavior of the rock mass is simulated as an anisotropic poroelastic continuum, without defining the precise geometry of the discontinuities, but using enriched constitutive models that consider the bedding plane dip angle.

We adopt the sign convention of geomechanics for stress and strain components throughout the paper, i.e., compression and compaction are positive. Finally, we present the stress evolution and stability analysis of the host rock in terms of total mean stress $\bar{\sigma}_m = \frac{\sigma_1 + \sigma_2 + \sigma_3}{3}$; effective mean stress $\bar{\sigma}_m = \sigma_m - ap$ and deviatoric stress $q = \frac{\sqrt{(\sigma_1-\sigma_2)^2+(\sigma_2-\sigma_3)^2+(\sigma_1-\sigma_3)^2}}{\sqrt{2}}$, where $\sigma_1$, $\sigma_2$ and $\sigma_3$ are principal stress components.

Given appropriate initial and boundary conditions, CODE_BRIGHT solves the formulation introduced in Eqs. (1) to (5) to determine primary unknowns: liquid and gas pressures and the displacement vector. The advective flow rate, diffusive flux and the stress tensor are then evaluated, respectively, from Eqs. (2), (3), and (5).

### 3.2 Geometry and model setup

We build a 2D plane strain model that reproduces a vertical cross-section of intact Opalinus Clay intersecting the injection borehole (Fig. 3). The model geometry extends 10 m on each side of the injection borehole in horizontal and vertical directions, indicated as $x$ and $y$, respectively, to avoid boundary effects. The bedding planes are inclined $45^\circ$ from the $x$ direction.

We hypothesize a horizontal injection well with a diameter of 0.086 m and a length of 0.2 m. Since the considered injection segment is substantially smaller than the model dimension, it resembles a point-like injection scheme. Thus, the borehole inclination plays a minor role from the perspective of simulation accuracy. To facilitate meshing, we adopt a horizontal borehole, which permits refinement around it while retaining the computational cost for a long-term simulation at an acceptable level. We discretize the model with a structured quadrilateral mesh consisting of 2560 elements. The mesh size progressively increases from 2 mm by 2 mm in the vicinity of the borehole up to 2.5 m by 2.5 m at the model boundaries. The refined mesh close to the injection segment allows accurate tracking of CO$_2$ intrusion into Opalinus Clay and the subsequent two-phase flow.

The vertical and minimum horizontal stresses coincide with the $y$ and $x$ directions, respectively (Fig. 3). We impose $\bar{\sigma}_1 \equiv \sigma_y = 6.5$ MPa and $\bar{\sigma}_3 \equiv \sigma_x = 2.2$ MPa at the borehole level. The vertical stress varies with depth with a lithostatic stress gradient of $25$ kPa/m, corresponding to the mean bulk density of the overlying layers of approximately $2500$ kg/m$^3$. The minimum horizontal stress distribution consistently follows the stress ratio $\bar{\sigma}_x/\bar{\sigma}_y = 0.34$ across the domain.

We set a pore pressure gradient of 10 kPa/m, with an initial fluid pressure of 2 MPa at the depth of injection. We neglect thermal effects and consider a constant and uniform temperature of 14 $^\circ$C.

We apply sinusoidal oscillations of the CO$_2$ pressure in the borehole at a mean pressure of 3 MPa, implying CO$_2$ injection occurs in a gas phase. The CO$_2$ pressure fluctuates in our reference model with an amplitude of $A_1 = 0.5$ MPa and a period of $T_0 = \frac{\pi}{2}$ d ($\approx 1.57$ d). We perform a sensitivity analysis to examine the potential impact of the injection pressure amplitude on the HM response of the shale. To this end, we take into account two other injection

![Fig. 3 Schematic view of the numerical model setting for CO$_2$LPIE, including the model geometry and boundary conditions. The injection segment of the borehole is illustrated in red. The results are plotted along the $x'$ and $y'$ directions, representing the directions parallel and perpendicular to the bedding planes, respectively. Dotted lines schematically show the bedding plane directions.](image-url)
scenarios: one with an amplitude lower by a factor of 2 and another one with an amplitude larger by a factor of 2 compared to the reference case, i.e., \( A_2 = 0.25 \text{ MPa} \) and \( A_3 = 1.0 \text{ MPa} \). In all simulations, we impose a constant vertical stress of 6.25 MPa at the top boundary and restrict any deformation perpendicular to the bottom and lateral boundaries. The hydraulic boundary conditions account for constant pressures of 1.9 MPa at the top and 2.1 MPa at the bottom boundaries and no-flow constraints on the lateral ones. We begin the simulation with an equilibration phase after imposing the initial and boundary conditions for fluid pressure and stress fields in accordance with in-situ measurements at the Mont Terri rock laboratory (Martin and Lanyon 2003; Corkum 2006).

3.3 Model parameters

The properties of Opalinus Clay used in our simulations are provided in Table 1. We define the orthotropic behavior of the shale using laboratory measurements performed by Makhnenko et al. (2017) and Makhnenko and Podladchikov (2018). An anisotropic intrinsic permeability tensor is used with 2.4 \( \cdot 10^{-20}\text{m}^2 \) and 0.8 \( \cdot 10^{-20}\text{m}^2 \) for the parallel- and normal-to-the-bedding directions, respectively (Marshall et al. 2004; Makhnenko et al. 2017). We assume that other hydraulic properties of the rock are isotropic. The relative permeability curves to both CO\(_2\) and brine phases are assumed to follow power-law functions of the brine saturation with a high exponent of 6 (Bennion and Bachu 2008; Kivi et al. 2022). The Biot coefficient anisotropy is estimated to be 5% and, therefore, is neglected, and the isotropic value of \( a = 0.76 \) reported for the initial in-situ conditions for CO\(_2\)LPIE is adopted (Makhnenko and Podladchikov 2018). Stress dependence of hydraulic and poromechanical properties of Opalinus Clay is not considered in the simulation of the pressure oscillations during periodic injections.

Mercury intrusion porosimetry provides essential information on the rock pore structure (Kuila and Prasad 2013). Application of this technique yields an interconnected rock porosity of 0.125 and a dominant pore throat size of 15 nm for Opalinus Clay. Based on estimates of the capillary pressure curve, we convert the measurements from the gaseous-liquid mercury to CO\(_2\)-brine capillary system using suitable interfacial properties. Given the average pressure and temperature of CO\(_2\)LPIE, a CO\(_2\)-brine interfacial tension of 50mN/m is employed (Kvanamme et al. 2007) and the contact angle on the mineral surface is set equal to 40° (Espinoza and Santamarina 2017). We fit the capillary pressure curves with the van Genuchten model (van Genuchten 1980)

\[
S_{el} = \frac{S_I - S_{el}}{S_{max,l} - S_{el}} = \left(1 + \left(\frac{p_{cap}}{p_0}\right)^{1/(1-m)}\right)^{-m}
\]

where \( p_0 \text{[ML}^{-1}\text{T}^{-2}] \) and \( m[-] \) are the gas entry pressure and shape parameter, respectively. \( S_{el} \) is the effective liquid saturation, normalizing the liquid phase saturation in its varying range from an irreducible saturation of \( S_{el} \) to a maximum value of \( S_{max,l} \). Assuming a high irreducible brine saturation of \( S_{el} = 0.5 \) for the shale, we approximate the best-fit van Genuchten parameters to be \( p_0 = 5\text{MPa} \) and \( m = 0.7 \). This model reproduces the capillary retention behavior of intact Opalinus Clay. Accounting for the effect of plausible rock heterogeneities at the URL scale, e.g., preferential entry pores for CO\(_2\), we examine the sensitivity of the system response by assuming different hydraulic properties of the host rock. For this purpose, we perform additional simulations by enhancing the permeability by two orders of magnitude, while at the same time, reducing the capillary entry pressure by a factor of 10.

| Property                              | Unit   | Value |
|---------------------------------------|--------|-------|
| Shear modulus along the bedding, \( G_p \) | GPa    | 0.63  |
| Young’s modulus along the bedding, \( E_p \) | GPa    | 1.7   |
| Young’s modulus perpendicular to bedding, \( E_n \) | GPa    | 2.1   |
| Poisson’s ratio along the bedding, \( \nu_p \) | –      | 0.35  |
| Poisson’s ratio perpendicular to bedding, \( \nu_n \) | –      | 0.32  |
| Biot coefficient, \( \alpha \)        | –      | 0.76  |
| Permeability along the bedding, \( k_p \) | m\(^2\) | 2.4 \( \cdot 10^{-20}\) |
| Permeability perpendicular to bedding, \( k_n \) | m\(^2\) | 0.8 \( \cdot 10^{-20}\) |
| Relative water permeability, \( k_{rw} \) | –      | \((S_{el})^6\) |
| Relative CO\(_2\) permeability, \( k_{rc} \) | –      | \((1-S_{el})^6\) |
| Porosity, \( \phi \)                  | –      | 0.125 |
| van Genuchten entry pressure, \( p_0 \) | MPa    | 5     |
| van Genuchten shape parameter, \( m \)  | –      | 0.7   |
In accordance with Henry’s law, the CO₂ solubility in water is linearly correlated with the CO₂ partial pressure. The Henry’s law constant is picked at the temperature and pressure range of the insitu experiment (Spycher et al. 2003). We neglect the effect of pore network tortuosity on the diffusive flux of aqueous CO₂ and assume an effective diffusion coefficient of $1.6 \times 10^{-9} \text{ m}^2\text{s}^{-1}$ that lies within the experimentally measured values for CO₂ diffusion in water (Tewes and Boury 2005).

4 Results

4.1 Reference case with amplitude $A_f=0.5 \text{ MPa}$

The applied cyclic CO₂ injection generates a slight brine overpressure that propagates into the caprock formation (Fig. 4a). The calculated liquid pressure distribution is distorted by the hydraulic anisotropy, advancing further along the bedding planes due to the fact that here the permeability is three times higher than the one normal to the bedding planes (Fig. 4a). The imposed gas pressure, which changes between 2.5 and 3.5 MPa, creates a brine overpressure that

![Spatial distribution after 20 years of cyclic CO₂ injection](image)

Fig. 4 Spatial distribution after 20 years of cyclic CO₂ injection of a liquid pressure and advance of the front of dissolved CO₂, using as threshold concentration twice as large as the initial value after 20 years of CO₂ injection; b total mean stress; c volumetric strain; and d deviatoric stress.
approaches 0.5 MPa around the borehole. Correspondingly, the capillary pressure (i.e., the difference between gas and brine pressures) does not build up to drive a meaningful desaturation and the free-phase CO$_2$ can only penetrate a few millimeters into Opalinus Clay. As a result, CO$_2$ flow appears to be controlled by molecular diffusion rather than advection. Additionally, although at negligible rates, the advecting brine promotes the spread of the dissolved CO$_2$ species (black dashed line in Fig. 4a). The diffusion-dominated CO$_2$ front expands isotropically because it is not affected by the preferential flow path along the bedding planes (black dashed line in Fig. 4a). It is noteworthy that gas transport has been the focus of various ongoing experiments conducted by the Mont Terri Consortium (see, e.g., Leupin et al. 2018; Heberling et al. 2022; Wüst et al. 2022).

The pore pressure buildup decreases the effective mean stress and, consequently, causes the rock to volumetrically expand (Fig. 4c). The expanded region is correlated with the pressurized area and, thus, propagates further away along the bedding planes. The poroelastic coupling perturbs the initial state of stress and induces compressive stresses, with an increase in the total mean stress of 0.3 MPa close to the injector (Fig. 4b). Similar to pore pressure propagation, the total mean stress and deviatoric stress are elongated along the bedding planes (Fig. 4b and d).

The applied periodic injection signal attenuates within a relatively short distance, i.e., tens of cm in the direction normal to the bedding, but advances significantly further along the bedding planes (Fig. 5). The distance at which the signal completely fades barely increases with time. In order to illustrate the behavior, simulation results are plotted at four moments within a single periodic cycle (see the insets in Fig. 5). Points $P_2$ and $P_3$ show two local maxima of the overpressure. The first one, marked with a dot, refers to the maximum gas pressure $p_g$, coinciding with the desaturated region around the well, while the second one refers to the maximum liquid pressure $p_l$. The region of desaturation is limited to a few cm around the well and does not propagate with time because of the high entry pressure of Opalinus Clay. In contrast, given the different permeability along and normal to the bedding planes, the pore pressure perturbation front advances with time in an anisotropic way, reaching 6 m and 3.5 m after 2 years of injection, and 14 m and 8 m after 20 years of injection along $x'$ and $y'$ directions, respectively.

The plots follow one cycle of the injection pressure evolution after 2 years and 20 years of periodic injection. The dots represent the maximum capillary pressure ($p_c = p_g - p_l$), which corresponds to the minimum water saturation $S_w$ for each curve. Given the van Genuchten parameters for Opalinus Clay in our reference model (see $p_0$ and $m$ in Table 1), both the magnitude and extent of the rock desaturation are quite small. CO$_2$ cyclically desaturates a region of approximately 80 mm width around the borehole (Fig. 6). Figure 6 represents the saturation degree evolution of the green and pink dots in Fig. 5a (i.e., parallel to the bedding) after 2 years and 20 years of injection. The desaturation starts when the liquid pressure becomes lower than the gas pressure. After 20 years, the liquid pressure does not show an evident variation at the point of interest, while the gas
pressure interestingly increases, resulting in enhanced pore network desaturation (Fig. 6b). However, final CO2 saturation is yet negligible. The increased CO2 pressure may be attributed to the fact that the pore-filling brine in the vicinity of the borehole has already become saturated with dissolved CO2, preventing further dissolution. This reduced dissolution rate gives rise to higher CO2 pressures. Additionally, it can be noted that the CO2 pressure evolution lags behind the one of the water pressure, which is a result of the higher compressibility of CO2 that leads to a delayed response to pressure changes (Vilarrasa et al. 2010b).

Pore pressure buildup induces an increase in the stress tensor components that results in a higher total mean stress (Fig. 7). The total mean stress changes are smaller, by a factor of around two, than the pore pressure changes (compare Figs. 7, 5). This implies that the effective mean stress reduces in all directions and the rock expands. It is also worth mentioning that the perturbed pore pressure and stress zones develop to similar extents after two years of injection (compare Figs. 7, 5). Interestingly though, unlike the pore pressure changes, over time, the induced stress curves do not reach significantly deeper into the formation. Therefore, the stress perturbation stays behind the advancing pressure front after 20 years.

4.2 Long-term rock stability and deformation

In the context of fluid injection, the integrity of the caprock could be negatively affected, resulting in leakage. CO2 could migrate into shallower formations or even escape to the atmosphere. A damage of the
clayrock should also be adverted in the case of the in-situ experiment at Mont Terri. Here, the relatively low mean overpressure of 1 MPa, as proposed for CO2LPIE, is not expected to induce sufficiently large changes in the effective stress to reach the failure conditions for Opalinus Clay (Fig. 8). For the rock stability, we interpolated the laboratory measurements in undrained triaxial compression conditions on shaly facies of Opalinus Clay. The Mohr–Coulomb failure criterion in terms of the deviatoric and mean effective stresses is expressed as follow (Meyer and Labuz, 2013)

\[ q = \frac{6 \cdot \sin(\phi)}{3 - \sin(\phi)} \sigma_m' + \frac{6c \cdot \sin(\phi)}{3 - \sin(\phi)} \]  

where \( c \) and \( \phi \) are the rock cohesion and friction angle, respectively. Our laboratory measurements yield a cohesion of 4.9 MPa and a friction angle of 24.7 degrees for Opalinus Clay.

The initial stress state is far from failure conditions because of the high cohesion of Opalinus Clay, so stability is guaranteed during the experiment. Note that the reduction in the effective mean stress is lower (by a factor of 2) than the mean overpressure of 1 MPa because pore pressure buildup induces compressive stresses. As a result, Opalinus Clay at the Mont Terri rock laboratory can stand a large pressure buildup without reaching failure conditions.

The displacements 1 m away from the injection well follow the trajectory that an observation well would follow, i.e., perpendicular to the bedding planes and parallel to the injection well (see inset in Fig. 9). Displacements remain in the sub-mm scale, even after 20 years of injection. The maximum changes occur in the vicinity of the injection segment. The region is relatively small due to the low permeability of Opalinus Clay, which limits pore pressure changes and changes in the effective stresses that induce deformation.

4.3 Sensitivity analysis of the amplitude of the periodic injection

We analyze the rock response to three source amplitudes of the periodic injection: 0.25 MPa, 0.5 MPa, and 1.0 MPa. In order to compare the results, the
pore pressure changes are normalized with respect to each amplitude, which we denote as \( p^* \). Figure 10 represents variations of the normalized pore pressure \( p^* \) after 20 years of injection at short distances from the injection well, both parallel and perpendicular to the bedding planes, for the three selected amplitudes. The signal amplitude along the bedding planes attenuates by 50% and 90% at distances of only 0.1 m and 0.2 m away from the injection well, respectively (Fig. 10a). The attenuation is higher normal to the bedding planes (Fig. 10b) compared to the direction parallel to the bedding. The shown curves correspond to a distance of 0.1 m and appear flattened in their minimum values because a slight desaturation takes place when brine pressure drops below CO\(_2\) pressure (recall Fig. 6). Note that injection at the lower amplitude of \( A_2 = 0.25 \text{MPa} \) does not desaturate the rock at a radius of 0.1 m. In contrast, injection at the highest amplitude \( A_3 = 1\text{MPa} \) leads to a more pronounced desaturation lasting for a longer period of time. The desaturation yet remains limited to some centimeters next to the borehole as none of the injection scenarios drains the rock even to a 0.2 m distance.

To evaluate the possibility of measuring signal fluctuations in-situ, we draw the same plot but for distances that reach up to 1 m (Fig. 11). Considering the amplitudes being on the order of 1 MPa, the periodic signal 0.5 m away from the injection well is calculated to be on the order of 1 kPa. As the distance from the well increases, the effect of shale anisotropy on the attenuation of the periodic signal and the lag time increases as well. This effect is more pronounced for the lag time, which presents a delay of half a day.

**Fig. 10** Temporal evolution of the normalized pressure \( p^* = (p - \bar{p})/A \) in the vicinity of the injection well shown for distances, \( D \), of 0.1 m, 0.2 m and 0.3 m away from the well.

**Fig. 11** Temporal evolution of the normalized pressure \( p^* = (p - \bar{p})/A \) around the injection well (shown for 0.5 m, 0.7 m, and 1.0 m away from the well); \( a \) parallel and \( b \) perpendicular to the bedding, for amplitudes \( A_1 = 0.5 \text{MPa}, A_2 = 0.25 \text{MPa} \) and \( A_3 = 1 \text{MPa} \), after 20 years of periodic injection.
4.4 Sensitivity analysis of hydraulic properties at the site scale

The presented model parameterized with laboratory data on cm-scale intact specimens provides preliminary insights into the HM response of Opalinus Clay to CO₂ injection. However, uncertainties grow when dealing with the rock mass behavior on the m to km scale. Particularly, the presence of flow discontinuities like fractures leads to higher intrinsic permeability and lower capillary entry pressure of the rock mass. Site- and regional-scale permeability of clay-rich shales can be up to two to three orders of magnitude larger than those inferred from laboratory experiments (Neuzil 2019). Furthermore, experimental measurements of relative permeability curves in low-permeability rocks are scarce, adding uncertainty to the model used in this study. In addition to our reference model, we simulate a scenario in which the intrinsic permeability is two orders of magnitude higher (i.e., ~ 10⁻¹₈ m²) and the capillary entry pressure is one order of magnitude lower than those in the reference model (i.e., 0.5 MPa). The relative permeability curves follow linear relationships with fluid saturations (i.e., exponents equal to one), which represents the least conservative case.

The high capillarity of the pore network and low permeability in the reference case hinder CO₂ intrusion into the caprock (Fig. 12a), while the low entry pressure and relatively high effective permeability allow CO₂ to enter and flow through the rock mass (Fig. 12b). In the former case, CO₂ dissolved into the brine spreads isotropically for almost 2 m away from the injector. For the latter case, the free-phase CO₂ spreads preferentially along the bedding, which promotes CO₂ dissolution along this direction. While the CO₂ front reaches a maximum distance of almost 2 m from the well along the bedding planes and 1 m normal to them, the extent of dissolved CO₂ ranges from almost 7 m along the bedding to 5 m normal to the bedding.

5 Discussion

Evaluation of the sealing capacity of anisotropic shaly caprocks, like Opalinus Clay, is complicated due to the presence of discontinuities that might provide preferential flow paths. Our numerical simulations...
of long-term periodic CO₂ injection into Opalinus Clay at the Mont Terri rock laboratory manifest the anisotropic HM response caused by the presence of bedding planes. In particular, the injection-induced overpressure follows the direction of the bedding planes, also promoting stress changes in this direction. The rock expands volumetrically and discontinuities may locally open along weak bedding planes, as they are found to possess lower tensile and shear strengths than the intact rock (Amann et al. 2018). Such an effect, although unlikely to occur during the experiment, as shown by the stability analysis (Fig. 8), could enhance intrinsic permeability and/or decrease the capillary entry pressure of the rock (Kim and Makhnenko 2020; Kivi et al. 2022) and might compromise the caprock integrity. In addition to the bedding, pore-scale shale heterogeneities may pose preferential conduits through which the injected CO₂ could penetrate and flow with further ease (Damians et al. 2020). However, even with a capillary entry pressure of one order of magnitude smaller than the one measured in the laboratory (pₜₐₓ = 0.5 MPa) and enhanced permeability by two orders of magnitude, the free-phase CO₂ can hardly penetrate 2 m into Opalinus Clay after 10 years of periodic CO₂ injection (Fig. 12b). If CO₂ does not advance in free phase, it dissolves in the pore fluid and spreads in the shale by the slower molecular diffusion process. The diffusive front advances uniformly and approaches a distance of about 2.5 m away from the borehole after 20 years of injection (black dashed line in Fig. 4a).

The preliminary insights gained from our coupled HM simulations assist in designing the CO₂LPIE experiment. In particular, to facilitate using the attenuation at the monitoring point for in-situ characterization of rock properties, set as a primary goal of the CO₂LPIE, appropriately locating the monitoring borehole is of high importance. We find that the imposed periodic oscillation attenuates rapidly, raising the necessity to locate the observation wells as close as possible to the injection well but still away from the borehole disturbed zone, at a safe distance to inhibit a short-cut between the boreholes. The amplitude of the periodic signal should be proportional to the distance to the injection well at which the monitoring wells will be finally drilled. Measuring and characterizing the geomechanical response of Opalinus Clay is less problematic, since drilling the monitoring borehole parallel to the injection well at a distance of 1 m would permit to accurately address the components of the strain tensor (Fig. 9).

The representability of our numerical simulations has been affected by some simplifying assumptions: (1) 2D plane-strain geometry, (2) high-exponent power-law model for the relative permeability curves, (3) constant poromechanical properties, permeability, capillary entry pressure, and irreducible water saturation with deformation, (4) linear elastic behavior of the rock matrix, and (5) neglecting chemical CO₂-brine-rock interactions. In more detail, the plane-strain model neglects fluid flow in the out-of-plane (parallel to the intermediate stress) direction. This simplification is thus anticipated to overestimate the generated overpressure and HM coupling along the bedding planes. Moreover, a true-triaxial evaluation of the stress alterations and rock deformation is of significance when dealing with strain-dependent mechanical and flow properties. Conducting multi-scale laboratory experiments on a carbonate specimen, Haghi et al. (2021) identified complex interactions between pore-scale deformations and two-phase flow mechanisms. They highlighted a systematically enhanced irreducible water saturation and decreased relative permeability with increasing the effective stress, as the pores become confined and flow paths get more tortuous. Nevertheless, similar coupling approaches in shales are underexplored, if considered at all, because of the challenging nature of such measurements in low-permeable rock. The considered power-law function in our study, although not calibrated, consistently reproduces the main relative permeability features of two shales obtained experimentally by Bennion and Bachu (2008), which is, to the best of our knowledge, the only (published) study of its kind. In that sense, CO₂ is found to remain immobile at saturations up to about 0.2—much larger than the attained CO₂ saturations in our reference model in the order of a few tenths of a percent (Fig. 6) -. On the other hand, the capillary entry pressure can be expected to decrease with pore radius increments during rock expansion, according to the Young–Laplace equation. Additionally, given that CO₂ dissolves into the formation pore fluid, geochemical reactions are expected. CO₂ dissolution in water generates carbonic acid (H₂CO₃) and decreases the pH of the liquid, which may lead to mineral dissolution and precipitation, potentially causing changes in rock porosity, permeability, stiffness and strength (Rohmer et al.
Our sensitivity analysis on rock properties partially addresses these non-linear capillary and flow effects in an ideally static pore structure framework. Nevertheless, we believe that the employed model parameterization approach constrains the simulation uncertainties to reasonable limits and provides a rational first-order approximation of the system response. To better characterize the formation and to control the evolution of the properties of the material, it is necessary to implement a continuous characterization method, taking into account different scales in time (from days to years) and space (from mm to tens of m). This is a key point that will be achieved by real-time calibration of the model parameters against field measurements during the CO₂LPIE.

6 Conclusions

We have performed numerical analyses of the CO₂LPIE experiment that will be conducted at Mont Terri rock laboratory to assist with its design. Coupled HM simulations of periodic CO₂ injection in Opalinus Clay are performed using a 2D plane-strain geometry over a long period of a few decades. Given the high entry pressure and low permeability of the material, CO₂ cannot penetrate and flow through the rock in free phase, unless the site-scale properties of Opalinus Clay substantially differ from laboratory measurements or geochemical interactions cause significant deterioration of the HM characteristics of the rock around the injection well. The injected CO₂ rather advances by molecular diffusion, reaching 1 m after 2 years, and 2.5 m after 20 years of injection. The periodic signal of the injection pressure rapidly attenuates, which requires the pore pressure monitoring wells to be located very close to the injection well. The pore pressure increase causes rock deformation and stress changes, which preferentially advance along the bedding planes, allowing to explore the anisotropic properties of Opalinus Clay in-situ. Measurements should be done by placing observation wells in orthogonal directions and not farther than a few tens of centimeters from the injector. The presented simulation results serve as the first approximation of the system response to periodic CO₂ injection and will be updated as more data is available and eventually compared with field measurements to gain insight on the sealing capacity of Opalinus Clay at the field scale.

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Declarations

Conflict of interest On behalf of all authors, the corresponding author states that there is no conflict of interest.

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References

Amann F, Le Gonidec Y, Senis M, Gschwind S, Wassermann J, Nussbaum C, Sarout J (2018) Analysis of acoustic emissions recorded during a mine-by experiment in an underground research laboratory in clay shales. Int J Rock Mech Min Sci 106:51–59. https://doi.org/10.1016/j.ijrmms.2018.04.021

Arts R, Eiken O, Chadwick A, Zweigal P, Meer L, van der Zinszner B (2003) Monitoring of CO₂ Injected at Sleipner Using Time Lapse Seismic Data. Greenhouse Gas Control Technologies - 6th International Conference https://doi.org/10.1016/B978-008044276-1/50056-8

Bachu S (2003) Screening and ranking of sedimentary basins for sequestration of CO₂ in geological media in response
Bandilla KW, Celia MA (2017) Active pressure management through brine production for basin-wide deployment of geologic carbon sequestration. Int J Greenhouse Gas Control 61:155–167. https://doi.org/10.1016/j.ijggc.2017.03.030

Bennion DB, Bachu S (2008) Drainage and imbibition relative permeability relationships for supercritical CO₂/Brine and H₂S/Brine systems in intergranular sandstone, carbonate, shale, and anhydrite rocks. SPE Reservoir Eval Eng 11(3):487–496. https://doi.org/10.2118/99326-PA

Bossart P, Meier PM, Moeri A, Trick T, Mayor JC (2002) Geological and hydraulic characterisation of the excavation disturbed zone in the opalinus clay of the mont terri rock laboratory. Eng Geol 66(1–2):19–38. https://doi.org/10.1016/S0012-825X(01)00140-5

Bossart P, Bernier F, Birkholzer J, Bruggeman C, Connolly P, Dewonck S, Fukaya M, Herfort M, Jensen M, Matray JM, Mayor JC, Moeri A, Oyama T, Schuster K, Shigeta N, Vietor T, Wieczorek K (2017a) Mont terri rock laboratory, 20 years of research: introduction, site characteristics and overview of experiments. Swiss J Geosci 110(1):3–22. https://doi.org/10.1007/s11242-016-0236-1

Bossart P, Jaeggi D, Nussbaum C (2017b) Experiments on thermo-hydro-mechanical behaviour of opalinus clay at mont terri rock laboratory, switzerland. J Rock Mech Geotech Eng 9(3):502–510. https://doi.org/10.1016/j.jrmge.2016.11.014

Boulin PF, Bretonnier P, Vassil V, Samouillet A, Fleury M, Bossart P, Jaeggi D, Nussbaum C, Jeanne P, Rutqvist J, Cappa F, Birkholzer J (2020) Complexity of fault rupture and fluid leakage in shale: insights from a controlled fault activation experiment. J Geophys Res: Solid Earth 125(2):1–19. https://doi.org/10.1029/2019JB017781

Bui M et al (2018) Carbon capture and storage (CCS): the way forward. Energy Environ Sci 11:1062–1176. https://doi.org/10.1039/C7EE02342A

Cavanagh AJ, Haszeldine RS (2014) The sleipner storage site: capillary flow modeling of a layered CO₂ plume requires fractured shale barriers within the utisra formation. Int J Greenhouse Gas Control 21:101–112. https://doi.org/10.1016/j.ijggc.2013.11.017

Cheng AHD (1997) Material coefficients of anisotropic poroelasticity. Int J Rock Mech Mining Sci Geomech Abstracts 34(2):199–205. https://doi.org/10.1016/S0148-9062(96)00055-1

Cheng AHD (2016) Poroelasticity. Book series: Theory and Applications of Transport in Porous Media, Vol.27 Springer, US

Corkum AG (2006) Non-Linear Behaviour of Opalinus Clay Around Underground Excavations. PhD thesis: Department of Civil and Environmental Engineering, University of Alberta, Canada.

Damians IP, Olivella S, Gens A (2020) Modelling gas flow in clay materials incorporating material heterogeneity and embedded fractures. Int J Rock Mech Min Sci 136:104524. https://doi.org/10.1016/j.ijrmms.2020.104524

Dewhurst DN, Raven MD, Shah SSBM, Ali SSBM, Giwelli A, Firs S, White C (2020) Interaction of super-critical CO₂ with mudrocks: impact on compositional and mechanical properties. Int J Greenhouse Gas Control 102:103163

Espinoza DN, Santamarina JC (2017) CO₂ Breakthrough—caprock sealing efficiency and integrity for carbon geological storage. Int J Greenhouse Gas Control 66:218–229. https://doi.org/10.1016/j.ijggc.2017.09.019

Favero V, Laloui L (2018) Impact of CO₂ injection on the hydro-mechanical behaviour of a clay-rich caprock. Int J Greenhouse Gas Control 71:133–141. https://doi.org/10.1016/j.ijggc.2018.02.017

Guglielmi Y, Nussbaum C, Jeanne P, Rutqvist J, Cappa F, Birkholzer J (2020) Complexity of fault rupture and fluid leakage in shale: insights from a controlled fault activation experiment. J Geophys Res: Solid Earth 125(2):1–19. https://doi.org/10.1029/2019JB017781

Haghi AH, Chalaturnyk R, Blunt MJ, Hodder K, Geiger S (2021) Poro-mechanical controls on spontaneous imbibition in earth materials. Sci Rep 11(1):1–11. https://doi.org/10.1038/s41598-021-82236-x

Heberling F, Albers H, Beielecke T, Deissmann G, Furche M, Geckes H, Hoyer EM, Joseph C, Liebscher A, Lüth S, Metz V, Müller K, Nowak U, Rebscher D, Schulte F, Steegborn F, Tietz T (2022) DR-D: The heterogeneity of the sandy facies of opalinus clay, Geophysical Characterization and Diffusion Study, Technical Meeting TM-39, 26. January 2022, virtual, Switzerland

Hildenbrand A, Schlömer S, Krooss BM (2002) Gas breakthrough-experiments on fine-grained sedimentary rocks. Geofluids 2(1):3–23. https://doi.org/10.1046/j.1468-8123.2002.00031.x

IEA GHG (2009) CCS Site Characterisation Criteri. IEA Greenhouse Gas R&D Programme

IPCC (2014) Climate change 2014: synthesis report. Contribution of working groups I, II and III to the fifth assessment report of the intergovernmental panel on climate change. IPCC, Geneva, Switzerland, p 151

Jaeggi D, Galletti M, Amacher F, Dunst R, Nussbaum C, Raselli R, Ringens M, Schefer S, Bossart P (2020) Gallery 2018: Excavation and geological documentation. Mont Terri Technical Report, TR2018–04

Kim K, Makhnenko RY (2020) Coupling between poromechanical behavior and fluid flow in tight rock. Transp Porous Media 135(2):487–512. https://doi.org/10.1007/s11242-020-01484-z

Kim S, Hosseini SA (2014) Above-zone pressure monitoring and geomechanical analyses for a field-scale CO₂ injection project in cranfield. MS Greenhouse Gases: Sci Technol 4(1):81–98. https://doi.org/10.1029/2017J B017781

Kivi IR, Makhnenko RY, Vilarrasa V (2022) Two-phase flow mechanisms controlling CO₂ intrusion into shaly caprock. Transp Porous Media 112:893–913. https://doi.org/10.1007/s11242-022-01748-w

Kuila U, Prasad M (2013) Specific surface area and pore-size distribution in clays and shales. Geophysical Prospecting, 61 (2-Rock Physics for Reservoir Exploration, Characterisation and Monitoring), 341–362

Kvamme B, Kuznetsova T, Hebach A, Oberhof A, Lunde E (2007) Measurements and modelling of interfacial tension for water + carbon dioxide systems at elevated pressures.
Leupin OX, Van Loon LR, Gimmi T, Wersin P, Soler JM (2018) Exploring diffusion and sorption processes at the mont terri rock laboratory (Switzerland): lessons learned from 20 years of field research. Swiss J Geosci 110(1):393–405

Makhnenko RY, Vilarrasa V, Mylnikov D, Laloui L (2017) Hydromechanical aspects of CO2 breakthrough into clay-rich caprock. Energy Procedia 114:3219–3228. https://doi.org/10.1016/j.ijep.2017.03.1453

Makhnenko RY, Podladchikov YY (2018) Experimental poroviscoelasticity of common sedimentary rocks. J Geophys Res: Solid Earth 123(9):7586–7603. https://doi.org/10.1002/2018JB015685

Marschall P et al (2004) Synthesis of Hydrogeological Investigations at the Mont Terri site (Phases 1 to 5). In: Heitzmann P editor (2004): Mont Terri Project – Hydrogeological Synthesis, Osmotic Flow. Reports of the Federal Office for Water and Geology (FOWG), Geology Series No. 6

Martin CD, Lanyon GW (2003) Measurement of in-situ stress in weak rocks at mont terri rock laboratory, Switzerland. Int J Rock Mech Min Sci 40(7–8):1077–1088

Meyer JP, Labuz JF (2013) Linear failure criteria with three principal stresses. Int J Rock Mech Min Sci 60:180–187. https://doi.org/10.1016/j.ijrmms.2012.12.040

Minardi A, Stavropoulou E, Kim T, Ferrari A, Laloui L (2021) Experimental assessment of the hydro-mechanical behaviour of a shale caprock during CO2 injection. Int J Underground Gas Control 106:103225. https://doi.org/10.1016/j.ijggc.2020.103225

Miocic JM et al (2016) Controls on CO2 storage security in natural reservoirs and implications for CO2 storage site selection. Int J Greenhouse Gas Control 51:118–125. https://doi.org/10.1016/j.ijggc.2016.05.019

Neuzil CE (2019) Permeability of clays and shales. Annu Rev Earth Planet Sci 47:247–273. https://doi.org/10.1146/annurev-earth-053018-060437

Nussbaum C, Bossart P, Amann F, Aubourg C (2011) Analysis of tectonic structures and excavation induced fractures in the opalinus clay, mont terri underground rock laboratory (Switzerland). Swiss J Geosci 104(2):187–210. https://doi.org/10.1007/s00015-011-0070-4

Olivella S, Carrera J, Gent A, Alonso EE (1994) Nonisothermal multiphase flow of brine and gas through saline media. Transp Porous Media 15:271–293. https://doi.org/10.1007/BF00613282

Olivella S, Gent A, Carrera J, Alonso EE (1996) Numerical formulation for a simulator (CODE_BRIGHT) for the coupled analysis of saline media. Eng Comput 13(7):87–112

Rebscher D, Vilarrasa V, Makhnenko RY, Nussbaum C, Kipfer C, Wersin P (2020) CO2LPIE Project—Combining in-situ, laboratory, and modelling work to investigate periodic CO2 injection into an argillaceous claystone. https://digital.cscis.es/bitstream/10261/224405/1/Rebscher_et_al_2020_CouFr ac_ext_Abstract_CO2LPIE.pdf

Ringrose PS, Mathesias R, Wright IW, Selama F, Hansen O, Bissell R, Saoula N, Midgley J (2013) The In salah CO2 storage project: lessons learned and knowledge transfer. Energy Procedia 37:6226–6236. https://doi.org/10.1016/j.ijep.2013.06.551

Roggero PR, Furre AK, Gilfillan SMV, Krevor S, Landrø M, Leslie R, Meckel T, Nazarian B, Zahid A (2021) Storage of carbon dioxide in saline aquifers: physicochemical processes, key constraints, and scale-up potential. Annu Rev Chem Biomol Eng 12:471–494. https://doi.org/10.1146/annurev-chembioeng-093020-091447

Rohmer J, Pluymakers A, Renard F (2016) Mechno-chemical interactions in sedimentary rocks in the context of CO2 storage: weak acid, weak effects? Earth Sci Rev 157:86–110

Rutqvist J, Tsang CF (2002) A study of caprock hydromechanical changes associated with CO2-injection into a brine formation. Environ Geol 42:296–305. https://doi.org/10.1007/s00254-001-0499-2

Rutqvist J, Birkholzer JT, Tsang CF (2008) Coupled reservoir-geomechanical analysis of the potential for tensile and shear failure associated with CO2 injection in multilayered reservoir-caprock systems. Int J Rock Mech Min Sci 45(2):132–143. https://doi.org/10.1016/j.ijrmms.2007.04.006

Rutqvist J, Vasco DW, Myer L (2010) Coupled reservoir-geomechanical analysis of CO2 injection and ground deformations at In Salah, Algeria. Int J Greenhouse Gas Control 4(2):225–230. https://doi.org/10.1016/j.ijggc.2009.10.017

Rutqvist J, Rinaldi AP, Cappa F, Jeanne P, Mazzoldi A, Urpi L, Guglielmi Y, Vilarrasa V (2016) Fault activation and induced seismicity in geological carbon storage – lessons learned from recent modeling studies. J Rock Mech Geotech Eng 8(6):789–804. https://doi.org/10.1016/j.rmege.2016.09.001

Spycher N, Pruess K, Ennis-King J (2003) CO2-H2O mixtures in the geological sequestration of CO2 I assessment and calculation of mutual solubilities from 12 to 100°C and up to 600 Bar. Geochimica et Cosmochimica Acta 67(16):3015–31. https://doi.org/10.1016/S0016-7037(03)00273-4

Tewes F, Boury F (2005) Formation and rheological properties of the supercritical CO2 water pure interface. J Phys Chem B 109(9):3990–3997. https://doi.org/10.1021/jp046019w

van Genuchten MT (1980) A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. Soil Sci Soc Am J 44(5):892–898. https://doi.org/10.2136/ssaj1980.03615995004400050002x

Verdon JP, Kendall JM, White DJ, Angus DA (2011) Linking microseismic event observations with geomechanical models to minimise the risks of storing CO2 in geological formations. Earth Planet Sci Lett 305(1–2):143–152. https://doi.org/10.1016/j.epsl.2011.02.048

Vilarrasa V, Bolster D, Olivella S, Carrera J (2010a) Coupled hydromechanical modeling of CO2 sequestration in deep saline aquifers. Int J Greenhouse Gas Control 4(6):910–919. https://doi.org/10.1016/j.ijggc.2010.06.006

Vilarrasa V, Bolster D, Dentz M, Olivella S, Carrera J (2010b) Effects of CO2 compressibility on CO2 storage in deep saline aquifers. Transp Porous Media 85(2):619–639. https://doi.org/10.1007/s11242-010-9582-z

Vilarrasa V, Rutqvist J, Rinaldi AP (2015) Thermal and capillary effects on the caprock mechanical stability at In salah.
Algeria Greenhouse Gases: Science and Technology 5(4):449–461. https://doi.org/10.1002/ghg.1486

Vilarrasa V, Makhnenko RY (2017) Caprock Integrity and induced seismicity from laboratory and numerical experiments. Energy Procedia 125:494–503. https://doi.org/10.1016/j.egypro.2017.08.172

Vilarrasa V, Makhnenko RY, Laloui L (2017) Potential for fault reactivation due to CO₂ injection in a semi-closed saline aquifer. Energy Procedia 114:3282–3290. https://doi.org/10.1016/j.egypro.2017.03.1460

Warszawski L et al (2021) All options, not silver bullets, needed to limit global warming to 1.5 °C: A scenario appraisal. Environ Res Lett. https://doi.org/10.1088/1748-9326/abfeec

Wüst R, Bauer W, Surkova M, De Cannière P, Yang T, Fink R, Elam WT, Grundl T, Gimmi T, van Loon T, Glaus M, Scherfer S, Leupin OX (2022) DR-B & DR-E Experiment: Long-term diffusion experiments in FMT – past and future with comparison to TBO experimental data. Technical Meeting TM-39, 26. 2022, virtual, Switzerland

Zappone A, Rinaldi AP, Grab M, Wenning QC, Roques C, Madonna C, Obermann AC, Bernasconi SM, Brennwald MS, Kipfer R, Soom F, Cook P, Guglielmi Y, Nussbaum C, Giardini D, Mazzotti M, Wiemer S (2021) Fault sealing and caprock integrity for CO₂ storage: an in situ injection experiment. Solid Earth 12:319–343. https://doi.org/10.5194/se-12-319-2021

Zhou Q, Birkholzer JT, Mehnert E, Lin YF, Zhang K (2010) Modeling basin- and plume-scale processes of CO₂ storage for full-scale deployment. Ground Water 48(4):494–514. https://doi.org/10.1111/j.1745-6584.2009.00657.x

Ziefle G, Matray JM, Maßmann J, Möri A (2017) Coupled hydraulic-mechanical simulation of seasonally induced processes in the mont terri rock laboratory (Switzerland). Swiss J Geosci 110(1):195–212. https://doi.org/10.1007/s00015-016-0252-1

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