3D hydro-mechanical modeling of shaly caprock response to CO₂ long-term periodic injection experiment (CO₂LPIE)

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ABSTRACT: Carbon capture and storage in deep geological formations is necessary to achieve a meaningful reduction of anthropogenic CO₂ emissions into the atmosphere. Given the buoyancy of the injected CO₂, it is essential to adequately characterize the sealing caprocks commonly comprised of clay-rich formations, including shales. If the inherent anisotropy of shales is not considered, model prediction errors will propagate with time and space. To limit errors, the accurate experimental laboratory measurements should be scaled up and the in-situ behavior of the caprock should be studied in detail. Underground rock laboratories (URLs) offer a unique opportunity to investigate the caprock sealing capacity at a few meters scale in a well-defined and well-monitored environment. This perspective applies to the CO₂ Long-term Periodic Injection Experiment (CO₂LPIE) at the Swiss Mont Terri URL. In the experiment, it is planned to inject gaseous CO₂ into Opalinus Clay, which is considered as a representative caprock for underground storage. Opalinus Clay shows large-scale anisotropic behavior due to the presence of bedding planes and heterogeneities. We numerically simulate the CO₂LPIE experiment using a 3D hydro-mechanical model and assuming linear poroelastic transverse isotropic behavior of the rock. We find that the CO₂ is unlikely to penetrate the rock in free phase, while the diffusive front of dissolved CO₂ in resident brine hardly propagates half a meter after two years of injection. The overpressure and induced deformation and stress changes preferentially develop along the bedding planes, although not sufficiently to lead to shear failure.

1. INTRODUCTION
To limit global warming to 1.5 °C, net carbon removal after 2050 should be targeted (IPCC, 2014). To reach this goal, it is critical to develop novel technologies and a promising approach is Carbon Capture and Storage (CCS). CCS is generally understood as the set of CO₂ capture from a large stationary source, transport to an injection site, and permanent storage in the subsurface (Benson and Cook, 2005). CO₂ density at the pressure and temperature of typical underground storage formations in sedimentary basins is approximately 65% of the in-situ brine density. As a result, the plume of the injected CO₂ will not only migrate outwards from the injection well, but also upwards until it finds a sealing layer called caprock (Tsang and Niemi, 2017). To assure long-term CO₂ trapping, it is of fundamental importance to properly characterize the caprock sealing capacity, commonly presented in terms of permeability, porosity, capillary entry pressure and relative permeability curves, and their evolution with time (Kaldi et al., 2011).

Several laboratory experiments analyzed the sealing capacity of intact caprock samples (Hildbrand et al., 2002; Boulin et al., 2013; Makhnenko et al., 2017; Rezaee et al., 2017; Minardi et al., 2021; and Kivi et al., 2022). However, upscaling these results to the reservoir scale and quantifying their evolution due to long CO₂ injection remain unclear. For example, at the Sleipner storage site,
Cavanagh and Haszeldine (2014) inferred an entry pressure for the interbedding shale layers being 35 times lower than that measured in the laboratory. This discrepancy may arise from the coupled thermo-hydro-mechanical response of the intact material and the existence of discontinuities on a larger scale. The presence of fault zones and bedding planes may result in localized deformation and fluid flow (Rutqvist and Tsang, 2002; Rutqvist et al., 2016). In addition, the injection generates an overpressure, which favors CO₂ intrusion into the caprock. This may lead to the expansion of the formation that changes the caprock sealing capacity (Rutqvist, 2012; Vilarrasa et al., 2015).

In-situ monitoring during several demonstration and industrial-scale CO₂ injection projects have provided fundamental insights into the caprock sealing behavior. However, given the complexity of managing CCS, the associated costs, and the resolution of monitoring equipment, there is a lack of detailed comprehensive information concerning the hydro-mechanical (HM) response of the caprock to the injected CO₂. From this point of view, underground rock laboratories (URLs) represent a connection between laboratory experiments and in-situ observations. Particularly, the Mont Terri rock laboratory in Switzerland, with its tunnel and niches system mainly excavated in Opalinus Clay, provides a unique, undisturbed environment to drill and instrument wells for the conduction of different CO₂ injection experiments. In this context, the CO₂ Long-term Periodic Injection Experiment (CO₂-LPIE) aims at assessing the caprock sealing capacity. The experiment plans to inject gaseous CO₂ into Opalinus Clay, with a mean overpressure of 1 MPa (above the initial 2 MPa pore pressure present in the rock laboratory) and a cyclic pressure variation. At the design stage, it is necessary to predict the values that measured properties may take and establish a starting point for the HM analysis. For this reason, we perform 3D-HM simulations of CO₂-LPIE. The 3D model allows obtaining more realistic predictions of the rock deformation and flow in the presence of bedding planes, and hence, is essential for the design of the experiment.

Along with the introduction of the experimental site, we present a synthetic description of the model and the representative parameters for Opalinus Clay. We evaluate the evolution of displacement and pressure fields inside the rock for a period of two years and inspect CO₂ flow mechanisms, as well as the stability of the rock mass and the bedding planes.

2. METHODOLOGY

2.1. Opalinus Clay at the Mont Terri URL

CO₂-LPIE will take place in the Mont Terri URL. The international research facility is located in the Northern part of the Swiss Jura Mountain Belt in the Canton Jura, close to the village of St-Ursanne (Bossart et al., 2017). The maximum overburden amounts to about 320 m. The research in Mont Terri started in 1996, since then the rock laboratory has been expanded in six different stages, the last of which was completed in 2019 (Figure 1). Despite having undergone several extensions, the Mont Terri URL remains almost entirely excavated within a single formation called Opalinus Clay.

Opalinus Clay is a claystone deposited around 174 Ma ago with a measured thickness of about 130 m (Hostettler et al., 2017). It is further subdivided into three lithofacies: sandy facies, carbonate-rich sandy facies, and shaly facies (Figure 1). The complex mineralogy of Opalinus Clay consists of carbonates, sheet silicates, and framework silicates. Sandy facies, compared with shaly facies, display a major quartz content, from about 30% to 20%; major calcite content, from about 15% to 7%; and less clay minerals, from about 20% to 65% (Thury and Bossart, 1999). Opalinus Clay has low permeability and porosity and high entry pressure that makes it a competent caprock for CO₂ storage (Thury and Bossart, 1999; Bossart and Thury, 2008; Bossart et al., 2017; Makhnenko et al., 2017; Makhnenko and Podladchikov, 2018).

Bossart et al. (2017) reported an overconsolidation ratio for Opalinus Clay of almost 5, which means that the maximum burial depth was around 1350 m. Formations at Mont Terri dip towards SSE with a variable angle. Opalinus Clay underlies the Passwang Formation (sandy limestones and shales) and overlies the Staffelegg Formation (limestones and marls with shaly intercalations). The uppermost facies of Opalinus Clay, where the CO₂-LPIE experiment is planned to be conducted, correspond to the sandy facies. CO₂-LPIE will inject CO₂ in the gaseous phase (mean pressure around 3 MPa and temperatures around 14 °C) into undisturbed rock (usually in roughly 10 m distance to the tunnel wall). The extent of mechanical and hydraulic perturbations and potential CO₂ penetration will be determined using appropriate monitoring tools installed in nearby monitoring boreholes. We will update our models during the experiment to provide improved understanding of the HM properties of Opalinus Clay at the experiment scale by reproducing the in-situ measurements. Our particular interest is in understanding potential CO₂ intrusion into shale, which may provide conclusive evidence for CO₂ leakage through the caprock at industrial CCS sites.
2.2. 3D numerical model

We build a 3D model of the CO2LPIE experiment using the fully coupled finite element code CODE_BRIGHT (Olivella et al., 1994; Olivella et al., 1996) extended and tested for CO2 injection (Vilarrasa et al., 2010a; Vilarrasa et al., 2010b; Vilarrasa et al., 2017). The code solves simultaneously the momentum balance and the mass conservation of CO2 and water. The advective fluxes of the two phases are calculated following Darcy’s law, with different values of permeability parallel and normal to the bedding (Table 1). We stipulate no transport of vapor in the gas phase and estimate the diffusion of CO2 inside the liquid phase with Fick’s law. The strains are then evaluated using the poroelastic theory (Detournay and Cheng, 1993; Cheng, 2016)

\[ \sigma = C \varepsilon + \alpha p, \]

where \( \sigma \) (Pa) is the stress tensor, \( \varepsilon \) (-) is the strain tensor, \( p \) (Pa) is the pore pressure, taken as \( p = \max(p_g, p_l) \), in which \( p_g \) and \( p_l \) are the gas and liquid pressures, respectively, \( \alpha \) (-) is the Biot effective stress tensor, hypothesized here to be a scalar for the sake of simplicity and lack of laboratory measurements, and \( C \) (Pa) is the elastic modulus tensor. We can also express the constitutive elastic behavior in terms of Biot effective stress (\( \sigma' = \sigma - \alpha p \))

\[ \sigma' = C \varepsilon. \]

Given the fact that Opalinus Clay shows a different behavior along and normal to the bedding planes (Thury and Bossart, 1999; Bossart and Thury, 2008; Makhnenko et al., 2017; Makhnenko and Podladchikov, 2018; Kim and Makhnenko, 2020), we impose a rotational symmetry on the axis normal to the bedding, leading to a transverse isotropic elasticity tensor (Cheng, 1997). The model is defined by five linear independent moduli: the Young’s moduli \( E_p \) and \( E_n \), the Poisson’s ratios \( \nu_p \) and \( \nu_n \), and the shear modulus \( G_n \), where the subscripts \( p \) and \( n \) refer to the directions parallel and normal to the bedding planes, respectively.

The model geometry comprises a 3D cube with an edge length \( L = 30 \) m (Figure 2), which is discretized with a total of 46,004 hexahedral finite elements variable in size: from 0.04-m sized elements around the injection well to 4.0-m sized elements near the model boundaries. In Figure 2, we draw the planes of transverse isotropy, with
a dip $\beta = 45^\circ$ representing the bedding planes. Note that the spacing between the bedding is not a parameter in the simulation, since we are using the transverse isotropic model.

Figure 2. Schematic view of the numerical model setting for CO$_2$LPIE, including the model geometry (30x30x30 m$^3$) and the injection well. The planes in orange represent the transverse isotropy directions (i.e., bedding planes) with a dip of $\beta = 45^\circ$. Plane v crosses the center of the injection well, it is vertical and forms an angle of 90$^\circ$ with the bedding planes. On the inset, we zoom around the injection well on Plane v. The dotted lines in orange show the inclination of the bedding planes along Plane v. The two representation points $A_p$ and $A_n$ belong to Plane v and are located at a distance of 0.1 m from the injection well, in the directions parallel and normal to the bedding, respectively.

For the initialization of the simulation, we hypothesize undisturbed conditions. At the depth of the well, we impose an initial liquid pressure of 2.0 MPa, varying with depth using a linear gradient of 0.01 MPa/m. The gas pressure is uniform and equal to the injection pressure. Regarding initial stresses, we impose $\sigma_x = \sigma_y = 6.5$ MPa, $\sigma_z = 4.0$ MPa, and $\sigma_{th} = \sigma_z = 2.2$ MPa at the injection depth, following Martin and Lanyon (2003) and Corkum (2006). The overburden stress corresponds to the maximum principal stress, which follows a linear distribution with a gradient of 0.025 MPa/m. This gradient results from an average density for Opalinus Clay of 2.45 g/cm$^3$ (Bossart and Thury, 2008). Before simulating gas injection, we perform a steady-state calculation to bring the pressure and stress field to an initial equilibrium.

The boundary conditions include no-flow and zero-displacement perpendicular to lateral boundaries. At the top, we impose constant vertical stress and pressure. At the bottom, we prevent vertical displacement and impose constant hydrostatic pressure. We simulate the injection phase by applying a sinusoidal variation of the gaseous CO$_2$ in the borehole. The injection pressure varies between 2.5 MPa and 3.5 MPa, which implies a mean pressure of 3 MPa (1 MPa higher than the hydrostatic), with a period of $\pi/2 \approx 1.57$ d. The injection well is defined as a hexagonal prism of length 0.2 m (along the x-axis) and hexagon cross-section (on the planeyz) with sides of 0.043 m. It is worth mentioning that with the time scale considered and the permeability and stiffness of Opalinus Clay (Section 2.3), the pressure and stress perturbations propagate no more than 2 m from the injection well. Thus, the simulation results are not affected by the model dimension.

In the insert of Figure 2, we zoom around the injection well in a vertical plane, called Plane v. This xz plane passes through the middle of the well. We display the simulation results at points $A_p$ and $A_n$, located at a distance of 0.1 m from the wall of the well in directions parallel and normal to the bedding, respectively.

Finally, we plot the results after two years of periodic CO$_2$ injection in terms of:

- pore pressure $p$;
- mean stress $P = \frac{\sigma_x + \sigma_y + \sigma_z}{3}$, where $\sigma_i$ are the stresses along the axes of our reference system;
- effective mean stress $P' = P - \alpha \rho p$;
- elastic volumetric strain $\varepsilon_{vol}$;
- deviatoric stress
  \[
  q = \frac{1}{\sqrt{2}} \left[ (\sigma_x - \sigma_y)^2 + (\sigma_y - \sigma_z)^2 + (\sigma_z - \sigma_x)^2 + 6(\tau_{xy}^2 + \tau_{yz}^2 + \tau_{xz}^2) \right],
  \]
  where the $\tau_{ij}$ are the tangential stresses in the reference system; and
- the Coulomb Failure Stress evolution $\Delta CFS = \Delta \tau + \Delta \sigma_{\tau} \cdot \tan(\phi)$, following Harris (1998). $\Delta \tau$ and $\Delta \sigma_{\tau}$ denote changes in shear and normal effective stresses compared to the initial conditions, respectively; and $\phi$ is the friction angle.

Here, the sign convention of geomechanics is adopted, i.e., positive for compressive stresses and strains.

### 2.3. Opalinus Clay parameters

We implement the 3D-HM modeling of the experiment using rock parameters derived from laboratory tests performed on Opalinus Clay specimens under representative in-situ conditions (Makhnenko et al., 2017; Makhnenko and Podladchikov, 2018; see Table 1 for a summary). The elastic parameters have been measured both parallel and normal to the bedding planes. Opalinus Clay has a porosity of 0.125. The intrinsic permeability equals $2.4 \cdot 10^{-20}$ m$^2$ and $0.8 \cdot 10^{-20}$ m$^2$ parallel and perpendicular to the bedding planes, respectively.
assume the Biot coefficient to be isotropic and equal to 0.76, neglecting the 5% anisotropy estimated by Makhnenko and Podlachikov (2018). The adopted values represent our first approximation of the rock mass behavior and agree well with those inferred from the twenty-years characterization of Opalinus Clay (e.g., Bossart and Thury, 2008).

The retention curve, which correlates the capillary pressure $p_c$ with the wetting phase saturation, is fitted with the van Genuchten power law (van Genuchten, 1980)

$$S_{el} = \frac{S_l - S_{rl}}{S_{m} - S_{rl}} = \left(1 + \left(\frac{p_c}{p_0}\right)^{1-m}\right)^m,$$

where $S_{el}$ (-) is the effective liquid saturation, $S_l$ (-) is the liquid saturation, $S_{rl}$ (-) is the residual liquid saturation and $S_{m}$ (-) is the maximum liquid saturation. The parameters $m$ and $p_0$ represent the shape function and the gas entry pressure, respectively. We presume an irreducible brine saturation of $S_{rl} = 0.5$ for Opalinus Clay and approximate the van Genuchten parameters to be $m = 0.7$ and $p_0 = 5$ MPa. Finally, the relative permeability curves of CO$_2$ and brine phases are assumed to be represented by power law functions of the corresponding phase saturations with an exponent of 6 (Bennion and Bachu, 2008; Kivi et al., 2022).

Table 1. Material properties used to describe the HM behavior of Opalinus Clay under CO$_2$ injection.

<table>
<thead>
<tr>
<th>Property</th>
<th>Unit</th>
<th>OPA</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young's modulus parallel to bedding, $E_p$</td>
<td>[GPa]</td>
<td>1.7</td>
</tr>
<tr>
<td>Young's modulus normal to bedding, $E_n$</td>
<td>[GPa]</td>
<td>2.1</td>
</tr>
<tr>
<td>Poisson's ratio parallel to bedding, $\nu_p$</td>
<td>[-]</td>
<td>0.35</td>
</tr>
<tr>
<td>Poisson's ratio normal to bedding, $\nu_n$</td>
<td>[-]</td>
<td>0.32</td>
</tr>
<tr>
<td>Permeability parallel to bedding, $k_p$</td>
<td>[m$^2$]</td>
<td>2.4·10$^{-20}$</td>
</tr>
<tr>
<td>Permeability normal to bedding, $k_n$</td>
<td>[m$^2$]</td>
<td>0.8·10$^{-20}$</td>
</tr>
<tr>
<td>Porosity, $\phi$</td>
<td>[-]</td>
<td>0.125</td>
</tr>
<tr>
<td>Gas entry pressure, $p_0$</td>
<td>[MPa]</td>
<td>5</td>
</tr>
<tr>
<td>Relative water permeability, $k_{rw}$</td>
<td>[-]</td>
<td>$(S_o)^6$</td>
</tr>
<tr>
<td>Relative CO$<em>2$ permeability, $k</em>{rc}$</td>
<td>[-]</td>
<td>$(S_c)^6$</td>
</tr>
<tr>
<td>Van Genuchten shape parameter, $m$</td>
<td>[-]</td>
<td>0.7</td>
</tr>
</tbody>
</table>

We assess the rock stability evolution during the experiment using the Mohr-Coulomb failure criterion, which is expressed in terms of the deviatoric and effective mean stresses as (Mayer and Labuz, 2013)

$$q = \frac{6\cdot \sin(\phi)}{3 - \sin(\phi)} P + \frac{6c\cdot \sin(\phi)}{3 - \sin(\phi)},$$

where $c$ (Pa) denotes the rock cohesion, with values for Opalinus Clay extracted from the literature (Table 2).

3. 3D-HM SIMULATION RESULTS

3.1. Pore pressure diffusion

The continuous cyclic CO$_2$ injection generates two pore pressure effects on the surrounded rock: a general increase of the mean value and a wave diffusion (Figure 3). After two years of injection, pore pressure variations at points $A_n$ and $A_p$ are found to attenuate by two orders of magnitude compared to that prescribed at the injection well. This is a consequence of the low hydraulic diffusivity of the rock, which significantly reduces the wave amplitude, even at a short distance from the well. If we consider the direction normal to the bedding planes, the amplitude is reduced to tens of kPa. Also the lag in time (or phase shift) is different in the two directions, with a delay from 11 h to 19 h for $A_n$ and $A_p$, respectively.

![Figure 3. Pore pressure imposed at the injection well (in grey) and pore pressure at 0.1 m from the injection well boundary (in brown) for a representative time period of seven days after two years of periodic injection. $A_n$ and $A_p$ refer to the directions of the pressure variations normal and parallel to bedding, respectively (inset in Figure 2) and $A_p^n \equiv A_p^o$ refers to the hydrostatic value of the pore pressure at the same points; here, they coincide since we choose points at the same depth.](image-url)

Apart from the wave diffusion, the injection also imposes a brine overpressure around the borehole of
approximately 0.044 MPa for $A_p$ and 0.027 MPa for $A_n$ after two years of injection. The high entry pressure of Opalinus Clay prevents the rock from desaturating, and the free-phase CO$_2$ penetrates into the rock only by a few millimeters. Therefore, the flow of CO$_2$ in our simulation is due to molecular diffusion inside the resident brine, with no significant gas advection.

3.2. Coupled hydro-mechanical effects

The pore pressure perturbation changes the stress field around the well (Figure 4a). We notice simultaneous growth of the mean value and a wave-form diffusion of the mean stress, similar to that observed for the pore pressure (Figure 3). The anisotropic behavior is still evident with higher variations parallel to the bedding planes, but this time on the order of a few kPa (0.0076 MPa and 0.0050 MPa for points $A_n$ and $A_p$, respectively). As for the phase of the waves, comparing pore pressure diffusion and mean stress (Figure 3 and Figure 4a), the curves for $A_p$ have the same phase while the curves for $A_n$ have an opposed phase. Finally, the injection of CO$_2$ causes an increase of the total stresses by 0.010 MPa for both $A_n$ and $A_p$.

The pore pressure buildup is higher than the induced poromechanical stress, as a result, the effective mean stress decreases (Figure 4b) and causes the rock to expand (Figure 4c). The larger changes in pore pressure and, thus, the effective mean stress in the direction parallel to bedding give rise to larger expansion in this direction.

3.3. Long-term stability of the rock mass

Having described the HM effect on the rock mass during the injection, we focus on assessing whether it contributes to a destabilization of the rock. After two years of injection, we find only minor changes in stresses on the $q$-$P'$ plane, which form a closed loop in response to each cycle of pressure variation (Figure 5). We notice a gradual decrease of the effective mean stress and an increase of the deviatoric stress. The stress loop dimension is larger in the direction parallel to the bedding, pointing to preferential perturbations of stress and pressure in this direction. However, the stress values are still far from the failure range provided by Bossart and Thury (2008) and shear failure along the bedding provided by Gräsle (2011), meaning that the rock failure is quite unlikely to take place during the experiment.

![Figure 4](image1.png)

Figure 4. a) Mean stress $P$, b) mean effective stress $P^*$, and c) volumetric deformation $\varepsilon_{v,\text{vol}}$ over time at 0.1 m from the injection well boundary for seven days after two years of periodic injection. The results for $A_n$ (in black) and $A_p$ (in orange) refer to the directions normal and parallel to bedding, respectively (inset in Figure 2). $A^0_p \equiv A^0_n$ (in brown) refers to the initial values in the same points; they coincide since we choose points at the same depth.

![Figure 5](image2.png)

Figure 5. Deviatoric stress vs mean effective stress plot for $A_n$ and $A_p$ after two years of periodic injection (inset in Figure 2). The trajectories remain far from the Mohr-Coulomb shear failure values for Opalinus Clay (Table 2). $A^0_p \equiv A^0_n$ refer to the initial values in the same points; they coincide since we choose points at the same depth. On the inset, deviatoric and mean effective stresses for $A_n$ (in black) and $A_p$ (in orange) are presented for the directions normal and parallel to bedding, respectively, for an entire cycle and after two years of periodic injection (from 731.82 d to 733.40 d).
3.4. Long-term stability of the discontinuity

We calculate the variations of the Coulomb Failure Stress (ΔCFS) with respect to its initial magnitude to assess the rock's tendency to fail along the bedding planes. The shear stress \( \tau \) and normal effective stress \( \sigma'_n \) acting on the bedding planes dipping at \( \beta = 45^\circ \) are determined by transforming the stress components from the Cartesian system (shown graphically on the Mohr circle, Figure 6a).

The ΔCFS fluctuates with time at points \( A_n \) and \( A_p \), consistent with cyclic evolutions of the pressure and stresses (Figure 6b). The ΔCFS returns positive values that follow the evolution of the effective stresses (Figure 4b). In particular, the effective stress state undergoes greater variations in \( A_p \) rather than in \( A_n \) and this leads to higher ΔCFS in \( A_p \), both for the mean value and the amplitude. The ΔCFS enhancements of a few hundreds of kPa after two years of injection reveal decreased stability. Since the bedding planes are not critically stressed, failure conditions are not reached.

4. DISCUSSION AND CONCLUSIONS

Simulation results show that both the intact rock mass and bedding planes of Opalinus Clay are far from failure conditions during the periodic injection in the CO2LPIE experiment. Thus, it is reasonable to assume an elastic behavior of the rock mass during CO2LPIE. However, there is a number of uncertainties that are associated with the experiment. First of all, the injection causes a cyclic evolution of stresses (Figure 5), which may degrade the rock surrounding the well if approaching the rock damage (microcracking) thresholds. During CO2LPIE, among other parameters, strains and pressures will be monitored, allowing for a continuous characterization of the material response and improved modeling capabilities and process understanding.

The coupled HM simulations show that bedding planes control pore pressure diffusion and stress changes. The caprock expands (Figure 4c), which may cause the porosity to increase and trigger indirect poroelastic effects (Figure 7), although not considered in our simulation. Another factor that may alter the porosity around the well is caused by the geochemical interactions with CO2 potentially promoting mineral dissolution and precipitation, which is evaluated in another study performed by CO2LPIE partners (Rebscher et al., 2022). Importantly, small porosity changes in caprock-like materials may result in significant permeability variations, governed by a power-law with exponents as high as 17 (Kim and Makhnenko, 2020). Geochemical interactions between CO2 and brine-saturated shales can also impose notable impacts on the capillary entry pressure of the rock (Rezaee et al., 2017). Dissolution-induced reduction of the capillary entry pressure may promote CO2 intrusion into Opalinus Clay. Consequently, the porosity alterations and the ensuing impacts on the HM behavior of the rock during the CO2LPIE experiment have yet to be addressed in more detail.
Given the unknowns still present in this phase of the experiment, it has not seemed pertinent to further complicate the selected model. Indeed, the characteristics of the rock mass are taken from a different part of the URL, since the niche for CO₂-LPIE is located in the more recently excavated gallery. For the initial stress state, we also used values prior to the construction of the last section of the tunnel (Martin and Lanyon 2003; Corkum 2006). It is of fundamental importance to accurately evaluate the stress field at the niche, in order to properly predict the behavior of the caprock during the injection of CO₂ (Rutqvist et al. 2008). We consider this work as a first approximation that will be updated with the data from CO₂-LPIE.

The main concern of the simulation is to evaluate the radial extent of the injected CO₂ at different times. In the long term, the CO₂ does not flow in free phase due to the high entry pressure, but it dissolves and diffuses uniformly into the pore water. Dominated by molecular diffusion, the rate of CO₂ transport is controlled by its solubility in the resident brine and the diffusion coefficient. We use the effective diffusion coefficient of dissolved CO₂ in brine, equal to 1.6·10⁻⁹ m²/s (Tewes and Boury 2005), drawing an upper bound limit for CO₂ diffusion through the tortuous pore network of tight shales. CO₂ solubility in water is linearly correlated with the CO₂ partial pressure in accordance with Henry’s law. We picked a Henry’s constant at the temperature and pressure range of Mont Terri URL, following Spycher et al. (2003). The diffusion in our simulation is uniform, driven by the dissolution of CO₂ inside the resident brine. Therefore, there is no flow of the gaseous CO₂ in free phase inside the rock. With these hypotheses, we took a threshold of the dissolved CO₂ inside the brine as the double of the initial one and estimated that CO₂ penetrates Opalinus Clay for 0.42 m and 0.52 m after one and two years, respectively. These values confirm that the behavior of Opalinus Clay is compatible with that of a caprock. On the other hand, this means that the monitoring wells must be positioned as close as possible to the injection well to be able to capture the mechanical and hydraulic perturbations.

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