Investigating the influence of mechanical anisotropy on the fracturing behaviour of brittle clay shales with application to deep geological repositories

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Abstract

Clay shales are currently being assessed as possible host rock formations for the deep geological disposal of radioactive waste. However, one main concern is that the favourable long-term isolation properties of the intact rock mass could be negatively affected by the formation of an excavation damaged zone (EDZ) around the underground openings. The goal of this thesis was to develop and validate a mechanically-based model of the deformation and failure process of a clay shale, namely Opalinus Clay (OPA), with particular focus on the influence of anisotropy on the short-term response of circular tunnels. To achieve this goal, a hybrid continuum-discontinuum numerical approach was developed in combination with new field measurements from the Mont Terri underground research laboratory. The response of OPA during the excavation of a full-scale emplacement (FE) test tunnel was characterized by geodetic monitoring of wall displacements, radial extensometers and longitudinal inclinometers. The deformation measurements indicated strong directionality induced by the combined effect of in-situ stress field and bedding planes striking parallel to the tunnel axis, with the most severe deformation occurring in the direction approximately perpendicular to the material layering. Computer simulations were conducted using a newly-extended combined finite-discrete element method (FEM/DEM), a numerical technique which allows the explicit simulation of brittle fracturing and associated seismicity. The numerical experimentation firstly focused on the laboratory-scale analysis of failure processes (e.g., acoustic activity) in brittle rocks, and on the role of strength and modulus anisotropy in the failure behaviour of OPA in tension and compression. The fracturing behaviour of unsupported circular excavations in laminated rock masses was then analyzed under different in-situ stress conditions. Lastly, the proposed modelling methodology was applied to the aforementioned FE tunnel to obtain unique insights into the EDZ formation process around emplacement tunnels for nuclear waste. The calibrated numerical model suggested delamination along bedding planes and subsequent extensional fracturing as key mechanisms of the damage process potentially leading to buckling and spalling phenomena. Overall, the research findings are already having a direct impact on the preliminary design process of an underground repository for nuclear waste in Switzerland.

1. Introduction

1.1. Problem statement

Clay shales are currently being assessed as host rocks for the underground disposal of solid radioactive waste. The key characteristics that make these argillaceous rocks suitable for nuclear waste storage include: very low hydraulic conductivity, low diffusion coefficients and good retention capacity for radionuclides, and potential for self-sealing of fractures [1]. However, the hydraulic and transport behaviour of the rock mass within the excavation damaged zone (EDZ) around the underground structures need to be routinely considered during performance assessment (PA) calculations [2]. Aside from directly affecting the stability of the excavation during construction, the EDZ is typically associated with a short-term permeability increase of several orders of magnitude, owing to the formation of newly connected porosity in response to fracturing of intact rock and shearing along structural features such as tectonic faults and bedding planes [3]. Upon support installation, time-dependent deformations lead to the loading of the EDZ fractures, which, in turn, causes the permeability in the EDZ to drop to almost intact rock values within a few years [4]. Furthermore, it has been shown that even an increase of the hydraulic conductivities in the EDZ by five orders of magnitude may not be relevant to the long-term safety as the low permeability of the intact rock in the far field effectively limits the flow of water into the EDZ. Nevertheless, the confidence in the aforementioned performance assessment calculations would increase significantly if a sound understanding of the EDZ generation process and behaviour could be obtained through a mechanically-based model of the fracture network (Fig. 1). Moreover, the assessment of long-term safety of a repository system, including the simulation of radionuclide transport towards the biosphere, would benefit greatly from the geometric information (e.g., damage shape and extension, fracture aperture and network interconnectivity) that could be extracted from such a numerical model for a range of different geomechanical scenarios. Based on these considerations, the ultimate goal of this study was to develop and validate a new robust numerical approach that could realistically capture the deformational and fracturing behaviour of shales and that could, therefore, aid the design and safety assessment of a deep geological repository (DGR) for radioactive waste.
1.2. State of the art and limitations of previous studies

1.2.1. Experimental studies

A large body of experimental evidence suggests that the mechanical behaviour of shales is heavily influenced by distinctive stiffness and strength anisotropy. This directionality in the mechanical response arises at different spatial scales within the rock due to a number of factors, including the laminated clayey micro-structure, the presence of foliation and bedding planes, and preferably-oriented rock mass features such as joints and tectonic faults. At the laboratory-scale, variation of elastic response, strength characteristics and failure mechanisms with varying angle between the principal stress directions and the specimen layering orientation is typically observed [5, 6]. At the field-scale, the stability of underground structures is highly dependent upon the relative orientation between the bedding orientation and the excavation axis [1, 7] (Fig. 1). In particular, catastrophic bending and buckling of layers around drifts [1], premature collapse of borehole walls [8, 7], and ground support and tunnel construction difficulties [9], have been reported when excavating in the direction parallel to the bedding plane strike.

Over the past 15 years, an extensive experimental research program has been conducted at the Mont Terri Underground Research Laboratory (URL) [10] on Opalinus Clay (OPA), a shale formation selected to potentially host a DGR for high-level waste in Switzerland. Owing to the local stratigraphy, most of the field studies to date have been mainly focused on the response of excavations aligned with the dip direction of bedding planes inclined at about 30° to 50° [3, 11, 12, 13, 14]. Conversely, according to the reference concept of the Swiss National Cooperative for the Disposal of Radioactive Waste (NAGRA), the emplacement tunnels of a high-level nuclear waste repository will be excavated in OPA at a depth ranging between 500 and 900 m under flat-lying bedding conditions [15]. Although the former case has been proven less prone to tunnel instabilities, it cannot be considered fully representative of the actual repository conditions, whereby the excavation axis striking parallel to the layering orientation is expected to play a key role in controlling the tunnel behaviour (Fig. 2).

1.2.2. Simulation studies

The large body of research for the experimental characterization of the EDZ in OPA has been accompanied by a number of modelling studies aimed at capturing the response of the rock mass observed in situ. The vast majority of numerical models adopted to date have been based on continuum mechanics principles using classic shear failure theory for elasto-plastic materials (Table 1). However, a number of experimental observations demonstrate that shales fail in a brittle manner under low-confinement conditions such as those characterizing the near field of excavations. In particular, rock mechanics tests on OPA indicate that the rock failure process, including the stress-strain response, fracture mechanisms and acoustic activity, is typical of that for brittle materials [6, 16, 17, 18]. Also, several field observations highlight strongly localized failure patterns in the form of brittle fracturing, including excavation-parallel extensional cracks [3, 7, 13]. As further discussed below, continuum-based modelling approaches may not provide the most appropriate computational framework when the progressive rock breakdown leads to an extended loss of continuity inside the material.

1.2.3. Available modelling techniques

The progressive degradation of material integrity associated with the rock deformation process, together with the influence of pre-existing discontinuities on the rock mass response, have represented a major drive for the development of new modelling techniques.

Conventional continuum mechanics formulations are based on theories such as plasticity and damage mechanics, which adopt internal variables to capture the influence of history on the evolution of stress and changes at the micro-structural level, respectively. Standard strength-based, strain-softening constitutive relationships cannot capture localization of failure as the lack of an internal length scale results in the underlying mathematical problem to become ill-posed [28]. To overcome these shortcomings, the description of the continuum must account either for the viscosity of the material, by incorporating a deformation-rate dependency, or for the change in the material micro-structure, by enhancing the mathematical formula-
Fig. 2: Characteristic fracture patterns with bending and buckling of layers observed around openings excavated parallel to the strike of bedding planes in OPA. (a) Microtunnel [7], (b) small borehole [1], (c) horseshoe-shaped access drift [1], and (d) hollow-cylinder experiment [16].

Table 1: Summary of selected modelling studies aimed at capturing the short-term EDZ formation process in Mont Terri OPA.

<table>
<thead>
<tr>
<th>Case study</th>
<th>Code</th>
<th>Dimensions</th>
<th>Anisotropy</th>
<th>Constitutive models</th>
</tr>
</thead>
<tbody>
<tr>
<td>ED-B tunnel [19]</td>
<td>Examine3D&lt;sup&gt;a&lt;/sup&gt;</td>
<td>3D</td>
<td>no</td>
<td>linear elastic</td>
</tr>
<tr>
<td>ED-B tunnel [20]</td>
<td>Phase2&lt;sup&gt;a&lt;/sup&gt;</td>
<td>2D</td>
<td>no</td>
<td>linear elastic</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>no</td>
<td>elasto-plastic</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>elastic-brittle-plastic</td>
</tr>
<tr>
<td>ED-B tunnel [21]</td>
<td>FLAC3D&lt;sup&gt;b&lt;/sup&gt;</td>
<td>3D</td>
<td>no</td>
<td>linear elastic</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>no</td>
<td>elasto-plastic</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>no</td>
<td>nonlinear elasto-plastic (SDM)</td>
</tr>
<tr>
<td>Security Gallery [22]</td>
<td>ELFEN&lt;sup&gt;c&lt;/sup&gt;</td>
<td>2D</td>
<td>no</td>
<td>elasto-plastic with joints</td>
</tr>
<tr>
<td>Security Gallery [23]</td>
<td>UDEC&lt;sup&gt;b&lt;/sup&gt;</td>
<td>2D</td>
<td>no</td>
<td>elasto-plastic with joints</td>
</tr>
<tr>
<td>EZ-B niche [13]</td>
<td>Phase2&lt;sup&gt;a&lt;/sup&gt;</td>
<td>2D</td>
<td>yes</td>
<td>elasto-plastic with joints</td>
</tr>
<tr>
<td></td>
<td>3DEC&lt;sup&gt;b&lt;/sup&gt;</td>
<td>3D</td>
<td>no</td>
<td>linear elastic</td>
</tr>
<tr>
<td>EZ-B niche [24]</td>
<td>FLAC3D&lt;sup&gt;a&lt;/sup&gt;</td>
<td>3D</td>
<td>yes</td>
<td>elastic</td>
</tr>
<tr>
<td>HG-A niche [25]</td>
<td>FLAC3D&lt;sup&gt;b&lt;/sup&gt;</td>
<td>2.5D</td>
<td>yes</td>
<td>elasto-plastic with ubiquitous joints</td>
</tr>
<tr>
<td>EZ-A niche [26]</td>
<td>FLAC3D&lt;sup&gt;b&lt;/sup&gt;</td>
<td>2.5D</td>
<td>yes</td>
<td>elasto-plastic with ubiquitous joints</td>
</tr>
<tr>
<td>FE tunnel (this work)</td>
<td>Phase2&lt;sup&gt;a&lt;/sup&gt;</td>
<td>2D</td>
<td>yes</td>
<td>linear elastic</td>
</tr>
<tr>
<td></td>
<td>Y-Geo&lt;sup&gt;d&lt;/sup&gt;</td>
<td>2D</td>
<td>yes</td>
<td>linear elastic</td>
</tr>
</tbody>
</table>

<sup>a</sup> Rocscience Inc.
<sup>b</sup> Itasca Consulting Group Inc.
<sup>c</sup> Rockfield Software Ltd.
<sup>d</sup> [27] and this work
Fig. 3: Fundamental principles of discontinuum-based codes. (a) Grain-based UDEC model [41], (b) PFC model [42, 43], (c) FEM/DEM model.
accounting for the presence of fracture networks [38]. The homogenization approach is typically limited by the fact that slip, rotations and separation as well as size effects induced by discontinuities cannot be explicitly captured. Alternatively, if the problem is controlled by a relatively low number of discrete features, special interface (or joint) elements can be incorporated into the continuum formulation [39]. This technique can accommodate large displacements, strain and rotations of discrete bodies. However, owing to the fixed interconnectivity between solid and joints and the lack of an automatic scheme to recognize new contacts, only small displacement/rotations along discontinuities can be correctly captured [40].

Discrete modelling techniques, commonly referred to as the Discrete Element Method (DEM), treat the material directly as an assembly of separate blocks or particles. Based on the adopted solution algorithm, DEM implementations are broadly divided into explicit and implicit methods. The term distinct element method refers to a particular class of DEMs that use an explicit time-domain integration scheme to solve the equations of motion for rigid or deformable discrete bodies with deformable contacts [44]. The most notable implementations of this method are represented by the Universal Distinct Element Code (UDEC/3DEC) [45] and particle-based codes such as the Particle Flow Code (PFC) [46] and Yade [47]. On the other hand, the best known implicit DEM is the Discontinuous Deformation Analysis (DDA) method [48]. Despite the fact that DEMs were originally developed to model jointed structures and granular materials, the application of DEM was subsequently extended to the case of systems where the mechanical behaviour is controlled by discontinuities that emerge as natural outcome of the deformation process, such as fracturing of brittle materials. As depicted in Fig. 3, the introduction of bonding between discrete elements allowed one to capture the formation of new fractures and, thus, extended the application of DEMs to simulate also the transition from continuum to discontinuum [42, 43, 49].

More recently, the original boundary between continuum and discontinuum techniques has become less clear as several continuum techniques are capable of dealing with emergent discontinuities associated with the brittle fracture process. In particular, the hybrid approach known as the combined finite-discrete element method (FEM/DEM) [50] effectively starts from a continuum representation of the domain by finite elements and allows a progressive transition from a continuum to a discontinuum with insertion of new discontinuities. Examples of FEM/DEM codes are given by the commercial software ELFEN [51] and the open-source program Y-Geo [27] adopted in this study and further described below.

### 1.3. Modelling approach

The modelling platform selected for this study was the FEM/DEM software named Y-Geo as it allows one to explicitly capture fracture and fragmentation processes in rocks [27]. Furthermore, the open-source nature of the computer code guarantees the flexibility necessary for adding newly-required modelling capabilities.

In Y-Geo, the progressive failure of rock material is modelled using a cohesive-zone approach, a technique first introduced in the context of the elasto-plastic fracturing of ductile metals [52] and then extended to quasi-brittle materials such as concrete and rocks [30]. During elastic loading, stresses and strains are assumed to be distributed over the bulk material (i.e., the continuum portion of the model), which is therefore treated as linear-elastic using constant-strain triangular elements (Fig. 3c). Impenetrability between elements is enforced by a penalty function method. Upon exceeding the peak strength of the material, the strains are assumed to localize within a narrow zone, known as the fracture process zone. Since
2. Theoretical and practical advancements

2.1. Modelling anisotropy of stiffness and strength

Shale formations are distinctively bedded materials with mechanical behaviour that is best described as transversely isotropic [54]. That is, the deformability of the rock can be considered isotropic within any plane normal to an axis of rotational symmetry coincident with the normal to the bedding plane orientation (Fig. 7a). Therefore, to describe the elastic response of OPA, a stress-strain constitutive law for transversely isotropic elastic solids was implemented in Y-Geo.

A number of experimental studies indicate a strong influence of textural anisotropy not only on the deformation response but also on the tensile as well as compressive strength of layered materials [5, 55, 56, 57]. The compressive strength generally exhibits a maximum value for configurations in which the loading direction is either perpendicular or, in certain cases, parallel to the plane of transverse isotropy (Fig. 7b). The minimum compressive strength is typically obtained for $\theta$ ranging between 30° and 60°. To capture this behaviour in a FEM/DEM model, two techniques, referred herein to as the discrete approach and smeared approach, respectively, were devised and compared.

With the discrete approach, the anisotropy of strength emerges as a natural property of an isotropic, homogeneous medium containing a distribution of finite-sized, cohesion-less fractures aligned with the plane of isotropy. Macroscopic shear failure along the layering direction, responsible for the reduced strength of Z-samples, is captured as a step-path surface resulting from the coalescence of the pre-existing cracks, which undergo tensile propagation from their tips (Fig. 8). For this
model, the variation of strength as a function of the layering orientation (Fig. 8b) can be analytically explained by the so-called sliding crack models (Fig. 8c). Using this technique, a realistic model of the mechanical behaviour of OPA at the laboratory-scale was obtained in terms of stiffness and strength anisotropy (Fig. 8c), as well as stress-strain behaviour and failure envelopes. However, since macroscopic shearing is due to linkage of a number of individual fractures whose individual growth direction does not coincide with the final fault orientation (Fig. 8a), the simulated failure plane is generally steeper than the bedding plane orientation and delamination of bedding planes cannot be captured. This behaviour is further aggravated in field-scale models, where layer spacing values on the order of tens of centimeters must be used due to computational constraints on the mesh resolution. At this scale, the crack coalescence mechanism cannot capture the slip zones parallel to critically oriented bedding planes.

Motivated by the shortcomings of the discrete approach, a new smeared approach was devised by assuming that the macroscopically observed strength anisotropy is induced by a similar anisotropy at the crack element level. Hence, directionality is directly introduced in the fracture model by imposing that the cohesive strength of each crack element is a function of the relative orientation, γ, between the crack element itself and the bedding orientation (Fig. 9a). In particular, the cohesive strength parameters, \( f_c \), \( G_{Ic} \), and \( G_{IIc} \), assume maximum and minimum values for \( \gamma = 0^\circ \) and \( \gamma = 90^\circ \), respectively. A simple linear variation with \( \gamma = 0^\circ \) between the minimum and maximum values for \( \gamma = 90^\circ \).
Fig. 9: Smeared approach for modelling strength anisotropy. (a) Linear variation of strength parameters with the angle, $\gamma$, between crack element and bedding. (b) Example of mesh combining Delaunay triangulation for the intra-layer material with edges preferentially aligned along the bedding plane direction.

The simulated stress-strain curves of Fig. 11 show that from point O to point A-A’ the response of the model is linear due to the elastic deformation of the continuum triangular elements. Modulus anisotropy is a direct consequence of the adopted transversely isotropic constitutive relationship. In the pre-peak stage (point A-A’ to B), the model exhibits non-linear behaviour due to material softening at the crack element level. The onset of non-linearity manifests itself first in the lateral strain curves ($A’= 55\%$ versus $A = 70\%$ of axial strain at peak), as crack elements start to yield in tension in the direction parallel to $\sigma_1$. The brittle post-peak behaviour (beyond point B) is characterized by the actual failure of crack elements with consequent macroscopic fractures propagating throughout the model (Fig. 10d). The simulated strength response (Fig. 13) exhibits the characteristic concave upwards, and parabolic in form, curve that has been typically observed in OPA [6] and other shales [5]. As shown in Fig. 12, the strength anisotropy emerges from the variation of specimen rupture mechanisms induced by the directionality introduced in the cohesive response of crack elements preferably aligned along the bedding plane direction. Unlike plane of weakness models [60], since no clear distinction between failure of the matrix and of bedding planes is made (Fig. 14), a smooth transition in the strength response with loading angle is reproduced.

2.2. Model validation

The FEM/DEM models (with smeared approach) were calibrated to match averaged values obtained through highly controlled unconfined compression tests and Brazilian tests on the shaly facies of the Mont Terri OPA [55]. Similarly to other discontinuum modelling approaches [42], the micromechanical input parameters of the FEM/DEM simulations were calibrated by comparing the emergent properties of the model to the relevant response of the tested rock (Table 2). To this end, an iterative, trial-and-error calibration procedure was adopted. The indirect tensile strength, $T$, and the uniaxial compressive strength, $UCS$, were chosen to characterize the short-term, undrained mechanical response of OPA and used as calibration targets. Since both macroscopic properties exhibit a strong dependence upon the orientation of bedding, P- and S-values of $UCS$ and $T$ were considered as well as the $UCS$ for bedding inclined at 45° (Z-sample).

The simulated stress-strain curves of Fig. 11 show that from point O to point A-A’ the response of the model is linear due to the elastic deformation of the continuum triangular elements. Modulus anisotropy is a direct consequence of the adopted transversely isotropic constitutive relationship. In the pre-peak stage (point A-A’ to B), the model exhibits non-linear behaviour due to material softening at the crack element level. The onset of non-linearity manifests itself first in the lateral strain curves ($A’= 55\%$ versus $A = 70\%$ of axial strain at peak), as crack elements start to yield in tension in the direction parallel to $\sigma_1$. The brittle post-peak behaviour (beyond point B) is characterized by the actual failure of crack elements with consequent macroscopic fractures propagating throughout the model (Fig. 10d). The simulated strength response (Fig. 13) exhibits the characteristic concave upwards, and parabolic in form, curve that has been typically observed in OPA [6] and other shales [5]. As shown in Fig. 12, the strength anisotropy emerges from the variation of specimen rupture mechanisms induced by the directionality introduced in the cohesive response of crack elements preferably aligned along the bedding plane direction. Unlike plane of weakness models [60], since no clear distinction between failure of the matrix and of bedding planes is made (Fig. 14), a smooth transition in the strength response with loading angle is reproduced.

2.3. Damage process around a circular excavation

The damage process around a 3-meter-diameter circular excavation in OPA with flat-lying bedding planes was simulated using the FEM/DEM smeared approach illustrated above. Although in the actual repository a tunnel liner is to be adopted to largely limit the development of the EDZ, in these simulations the rock mass was left unsupported. The in-situ stress fields reported in Table 3 were adopted.
Fig. 10: Comparison of simulated fracture patterns with typical experimental observations [59, 23].

Fig. 11: Simulated stress-strain behaviour under uniaxial compression for (a) the P-sample and (b) S-sample, also showing counts of yielded/broken crack elements as columns.

Table 3: In-situ stress conditions applied to the excavation models.

<table>
<thead>
<tr>
<th>Case</th>
<th>$\sigma_v$ (MPa)</th>
<th>$\sigma_h$ (MPa)</th>
<th>Stress Ratio, $K_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>2.0</td>
<td>2.0</td>
<td>1.00</td>
</tr>
<tr>
<td>b</td>
<td>2.5</td>
<td>1.5</td>
<td>0.60</td>
</tr>
<tr>
<td>c</td>
<td>1.5</td>
<td>2.5</td>
<td>1.67</td>
</tr>
</tbody>
</table>

2.3.1. Isotropic in-situ stress field

Failure around the excavation boundary initiates in the haunch area at angles $\alpha$ approximately equal to $\pm 45^\circ$ and $\pm 135^\circ$ in the form of shear-dominated fractures along the bedding planes (Fig. 15a). This distinctive location of failure and fracturing behaviour can be explained by the presence of bedding planes inclined at an angle of about 30 to 60° to $\sigma_1$, which drastically reduces the strength of the rock resulting in premature bedding slip. The slippage of bedding planes in the haunch area causes a local perturbation in the stress field which results in the nucleation of extensional fractures in the direction perpendicular to the layering (Fig. 15b). As the delaminated layers tend to bend and slide past each other, brittle spalling is promoted in the tunnel sidewalls. The failure of rock in the sidewalls causes in turn the deflection and inwards sliding of
Fig. 12: Influence of bedding orientation on the UCS response. (a) Simulated fracture patterns for different loading orientations. (b) Rosette plots of the relative distribution of failed crack elements orientation.

Fig. 13: Simulated UCS and $E$ as a function of $\theta$. Dashed error bars indicate the ranges of experimental UCS values from Table 2.

Fig. 14: Inclination of macroscopic failure plane versus dip of specimen bedding. Indicated is also the relationship between mesh topology, orientation of bedding planes and fractures. Shown is also a typical shear failure observed during compression tests on Z-samples of OPA with bedding plane orientation indicated by a white line [6].

other unsupported layers of rock in the back and invert. The final damaged zone tends to assume a rectangular shape with
Fig. 15: FEM/DEM simulation results of the excavation failure sequence for the case $K_0 = 1.0$. Principal stress trajectories are indicated as cross icons with the long and short axis oriented as $\sigma_1$ and $\sigma_3$, respectively.
long walls perpendicular to the layering and short walls parallel to the layering (Fig. 15c). Although buckling of layers can be observed in the back and invert, the potentially catastrophic deepening of the fractured zone is prevented by the development of stress arching, as can be inferred by the contour of \(\sigma_1\). The analysis of the associated total displacement, \(\delta\), contour (Fig. 16) indicates that, at close proximity to the opening, the convergence of the tunnel is governed by rock mass fracturing and bulking resulting in large deformations, while at a distance from the excavation, the rock mass behaves elastically.

The failure mechanisms here simulated are, at least qualitatively, supported by a number of field or laboratory observations in excavations in laminated shale formations. In particular, the characteristic shear failure of bedding planes has been observed in OPA during hollow cylinder experiments [16] (Fig. 16(inset)), and around boreholes, microtunnels and drifts at the Mont Terri URL [1, 7]. Also, the importance of weakness planes in controlling the rock mass behaviour and the stability of underground openings is confirmed by observations from the construction of a hydroelectric tunnel in laminated sedimentary formations [9]. Characteristic square-shaped fractured zones have also been reported in the hydrocarbon exploration industry when drilling horizontal boreholes in laminated shales [8]. Furthermore, brittle failure in the form of extensional fractures parallel to the tunnel walls have been typically observed around excavations at the Mont Terri URL [3, 13].

### 2.3.2. Anisotropic in-situ stress field

In the case of anisotropic in-situ stress conditions, extensional brittle fracturing can be observed in the sidewalls for both cases (Fig. 17). However, the interaction between newly-created shear fractures and in-situ stress field results in sensibly different stress redistributions, which in turn deeply affect the final shape and extent of the EDZ. For \(K_0 = 0.60\), the lateral growth of bedding plane delamination is suppressed by the increase in shear strength due to the maximum principal stress locally oriented in the direction perpendicular to the layering. Consequently, the flow of \(\sigma_1\) around the hole tends to promote further failure in the roof and invert resulting in a vertically elongated damaged zone. Conversely, for \(K_0 = 1.67\) the lateral development of bedding slippage from the haunch is greatly enhanced by the orientation of the far field stresses with \(\sigma_3\) oriented perpendicular to the direction of fracture propagation. The fracture-induced stress redistribution limits the flow of \(\sigma_1\) around the back and invert. Therefore, the vertical development of EDZ is reduced in favour of further bedding slippage in the horizontal direction up to a depth of \(2r\) from the haunch area. Based on the above results, both fracture patterns differ from damaged zones typically observed in massive isotropic rocks whereby spalling is generally observed at the intersection of the minimum principal stress axis and the hole boundary.

### 3. Verification of the proposed solution

Recently, a test tunnel was excavated at the Mont Terri URL as part of a long-term research project (“Full-scale Emplacement (FE) experiment”) aimed at studying the thermo-hydro-mechanical effects induced by the presence of an underground repository for high-level radioactive waste. Despite several important differences between the Mont Terri URL and the actual repository site candidates (e.g., depth, stress state and tectonic imprint), the FE experiment offered the opportunity to analyze for the first time the behaviour of OPA under geometric (i.e., same tunnel shape and dimensions) and structural-geological (i.e., tunnel oriented parallel to the bedding strike) conditions similar to those of planned repository tunnels [2, 15]. The 50 m long FE tunnel was excavated full-face from northeast to southwest direction starting from the FE niche and it is entirely located within the shaly facies of the OPA formation (Fig. 18). The excavated and final tunnel diameter (including lining) were approximately equal to 3.0 and 2.7 m, respectively (Fig. 19). At the location of the FE tunnel, the average bedding orientation of 139/33 results in the excavation axis approximately parallel to the strike of bedding planes.

To quantitatively characterize the rock mass response, an extensive monitoring program was carried out before, during, and after the construction of the tunnel. The monitoring campaign included geodetic monitoring of tunnel wall displacements, radial multi-point extensometers, inclinometers, and pore water pressure measurements. Subsequently, the deformational behaviour observed in the field was analyzed using a calibrated FEM/DEM model in order to obtain unique insights into the formation process of the EDZ.
3.1. Short-term deformational response

The ground vertical displacement, $\delta_v$, above the crown of the FE tunnel was continuously monitored by inclinometers permanently installed in two 45 m long boreholes drilled sub-parallel to the tunnel axis. A sharp increase in $\delta_v$ was usually recorded at about $3 - 4$ m ($1.0 - 1.3D$) ahead of the excavation face (Fig. 20a). The progressive reduction of distance between isolines indicates that the deformation in the crown tended to stabilize as the excavation face moved further away from the sensor. The vertical displacement recorded above the excavation face was ranging between 29 and 43% of the maximum short-term (i.e., time-dependent deformation excluded) vertical displacement experienced at the given section. Inclinometers data were used to validate the estimate of the tunnel wall pre-convergence obtained from numerical tunnel longitudinal profiles.

The short-term tunnel wall displacements measured between
sections C1 and C5 (Fig. 19) were averaged in order to create an experimental model to be used as a reference for the numerical simulations (Fig. 20b). The anisotropy in the radial displacement field indicates a strong influence of the rock textural anisotropy, rock mass fabric (e.g., preferably-oriented tectonic shears), and in-situ stress orientation on the tunnel behaviour. Furthermore, the high displacements recorded at P5 ($\delta = 40$ mm) appear to cause a substantial deviation of the strain field from polar symmetric conditions, thus suggesting possible heterogeneities within the rock mass, a non-circular tunnel geometry, or a poorly supporting shotcrete invert. The average relative closure values varies between a minimum of 0.5% and maximum of 2.0% along line 1-3 and 1-5, respectively. Overall, this analysis shows that larger tunnel wall closures tended to occur along lines oriented approximately in the direction perpendicular to the bedding plane orientation (i.e., P5-P3, P2-P5, P1-P5).

3.2. FEM/DEM simulations

A core replacement technique was implemented to simulate the excavation advance and to capture the supporting effect of the tunnel face in the 2D FEM/DEM model. The amount of tunnel wall deformation that occurred prior to support installation was estimated from a numerical longitudinal displacement profile of the tunnel and validated with the inclinometer measurements (Fig. 20a). The simulated displacements were then reduced by the estimated percentage (i.e., 55%) for direct comparison with field measurements. The choice of cohesive strength parameters was initially based on the laboratory-scale calibration process carried out in Section 2.2 for the shaly facies of the Mont Terri OPA [55]. Given the coarser spatial discretization of the field-scale models, the input strength parameters were then re-calibrated to match the averaged short-term tunnel wall displacements measured between TM 10.6 and 34.3 (Fig. 20b). Overall, the point-wise comparison of numerical
Fig. 19: Simplified longitudinal cross section of the FE tunnel showing the installed support measures, the convergence measuring sections (C0-C9), and the location of radial extensometers (E1 and E2).

Fig. 20: Deformational response of the FE tunnel. (a) Evolution of ground vertical displacement measured by one of the two inclinometer chains and represented for different positions of the excavation face. The vertical displacement recorded at the excavation face and the corresponding maximum short-term values are indicated by orange and green circles, respectively. (b) Displacement vector plot of short-term values averaged in longitudinal direction from TM 10.6 to TM 34.3. Shaded areas indicate the range of variation at each point based on minimum and maximum value of x and y components. A 20× exaggeratedly deformed excavation profile is qualitatively indicated by a black dashed line.
Fig. 21: Comparison of simulated tunnel wall deformation with averaged field measurements. (a) Evolution of δ at five points along the tunnel boundary. Error bars indicate the range of variation of the correspondent field measurements (Fig. 20b). (b) Convergences associated with the displacements of the elastic model, of the FEM/DEM analysis, and the average field measurements (Fig. 20b).

and experimental values was, to a certain degree, skewed by the heterogeneous response of the actual excavation (possibly due to the presence of tectonic faults), which the homogenous model had no means to capture (Fig. 21a). Therefore, an alternative comparison was carried out by considering the relative displacements between the target points in lieu of absolute displacements. To this end, a comparison between measured and simulated convergences is shown in (Fig. 21b). As expected, values obtained from a preliminary elastic analysis substantially under-predicted the field measurements, thus suggesting the fact that linear elasticity was not the main source of deformation. Conversely, an overall good fit of the experimental data was provided by the FEM/DEM model, which reproduced well the anisotropic response of the rock mass.

3.2.1. Simulated EDZ formation process

Failure around the excavation boundary initiates at approximately $0^\circ \leq \theta \leq 15^\circ$, $120^\circ \leq \theta \leq 195^\circ$, and $300^\circ \leq \theta \leq 360^\circ$ in the form of shear-dominated fractures along the bedding planes (Fig. 22a). As the simulation progresses, the slippage of bedding planes causes a local perturbation in the stress field which results in the nucleation of strain-driven, Mode I fractures in the direction perpendicular to the layering (Fig. 22b). Further rock mass deconfinement triggers further delamination of bedding planes (Fig. 22c) with formation of wing-shaped fractured zones that tend to extend out in the direction parallel to the bed-ding to a distance of about 3 m from the sidewalls. After installing the support, the propagation of damage away from the opening is suppressed in favour of fragmentation in close proximity to the excavation boundary until new equilibrium conditions are reached (Fig. 22d).

The redistribution of compressive stress in response to the tunnel excavation (Fig. 23) is influenced by the in-situ stress anisotropy as well as the characteristic fracture pattern with bedding-parallel discontinuities and a heavily fractured zone around the tunnel. The lateral extension of the EDZ due to bedding delamination is suppressed by the re-orientation of $\sigma_1$ in the direction perpendicular to bedding. In proximity to tunnel boundary, bedding plane slippage promotes a drastic reduction of confining stress, $\sigma_3$, with low to moderately negative values responsible for the observed extensional fracturing.

At a distance from the excavation, the rock mass behaves elastically and therefore small strains, induced by the stress redistribution around the damaged zone, are simulated. Due to the highly anisotropic rock mass response, this distance varies between a minimum of 0.5 m to a maximum of 3 m in the direction parallel to bedding and in the sidewalls, respectively. Furthermore, elastic deformations of higher intensity are captured in the direction sub-perpendicular to the bedding orientation due to the high rock compressibility in the said direction. The radial extension of the fractured zone in the direction parallel (i.e., along EXT-01) and perpendicular (i.e., along EXT-02) to bedding is equal to approximately 0.5 and 1.5 m. These estimations are consistent with the possible experimental limits of the EDZ estimated from pore water pressure measurements and equal to 2.3 and 2.8 m, respectively [61]. In the direction parallel to bedding, the FEM/DEM model predicts a relatively smooth decrease in radial deformation with increasing distance from the tunnel wall (Fig. 24b). This behaviour reflects the general absence of fracturing and consequent deformation behaviour associated mainly with the elastic redistribution of stress around the tunnel. Conversely, a number of displacement jumps are simulated in the direction perpendicular to bedding due to extensive loss of material continuity occurring in close proximity to the excavation boundary (i.e., within about 1.0 m).
4. Concluding remarks

The safety assessment procedure for DGRs should be based on a sound understanding of the mechanisms involved in the development of damage around underground excavations. In this context, the goal of this thesis was to improve the current knowledge of the process that leads to the formation of an EDZ fracture network in clay shales, a distinctively anisotropic rock type currently being assessed as potential host formation in several countries. To achieve this goal a combination of innovative modelling techniques and field measurements from the Mont Terri URL was employed.

New modelling procedures and associated algorithms were developed for the combined finite-discrete element method (FEM/DEM) and validated against experimental results. In particular, the characteristic stiffness and strength anisotropy of shales was captured by: (i) smearing the transversely isotropic elastic deformation of the material in the continuum formulation of FEM/DEM, (ii) preconditioning the triangular mesh along the bedding plane direction, and (iii) developing a directional cohesive fracture formulation to reproduce the variation of failure mechanisms and strength response as function of the layering orientation. Using this approach, the contribution of different failure mechanisms to the EDZ formation process around circular tunnels was studied. It was possible to observe that, for tunnels excavated parallel to the bedding strike, failure initiates with shearing along bedding planes and later evolves with extensional fracturing in the direction perpendicular to the layering. Spalling and buckling failures were also simulated and shown to be promoted by the delamination of bedding planes. Under anisotropic in-situ stress states, the combination of material intrinsic anisotropy and anisotropy induced by fracturing results in fracture patterns and damage locations substantially different than those typically observed in massive isotropic rocks in similar stress conditions. Finally, thanks to the participation in the FE experiment of the Mont Terri Project, computer simulation results were integrated with deformation monitoring data recorded in situ, thus allowing to validate the proposed numerical approach and to obtain, for the first time, a quantitative representation of the EDZ development in OPA.

The methodology developed in this thesis has been finding direct application in the site-selection process and preliminary design of a geological repository for radioactive waste in Northern Switzerland. Numerical analyses using FEM/DEM have been employed to perform sensitivity studies aimed at assess-
Stress, $\sigma_1$, (MPa)

Minimum Principal Stress, $\sigma_3$

Maximum Principal Stress, $\sigma_1$

Stress, $\sigma$ (MPa)

-2 0 5 10 15

Fig. 23: Final stress distribution with principal stress directions indicated by short straight lines.

Radial Distance from Tunnel Wall (m)

Radial Displacement, $\delta$ (mm)

Total Displacement, $\delta$ (mm)

EXT-01
EXT-02

Fig. 24: (a) Total displacement field around the FE tunnel corresponding to the fracture pattern and stress distribution of Fig. 22d and Fig. 23, respectively. Visual comparison of the simulated fracture network with the breakout observed in the HG-A microtunnel [7]. (b) Radial displacement along lines EXT-01 and EXT-02.

ing the spectrum of expectations with regard to the creation and evolution of the EDZ under different geomechanical scenarios [62]. Also, information about the excavation-induced porosity and fracture inter-connectivity has been extracted from the FEM/DEM models and used as input for long-term simulations of fluid flow and radionuclide transport. Furthermore, it is noteworthy that the numerical model of the clay shale mechanical behaviour developed for this thesis can be readily applied
to other related rock engineering problems involving fracture propagation in layered rocks, including borehole stability assessment and hydraulic fracturing simulation [63].

References


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