Three-dimensional FDEM numerical simulation of failure processes observed in Opalinus Clay laboratory samples

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A R T I C L E   I N F O

Article history:
Received 4 September 2014
Received in revised form 16 October 2014
Accepted 20 October 2014
Available online 7 November 2014

Keywords:
Three-dimensional (3D) hybrid finite-discrete element method (FDEM)
Intermediate principal stress
Discrete element methods
True triaxial behaviour
Failure envelope

A B S T R A C T

This study presents the first step of a research project that aims at using a three-dimensional (3D) hybrid finite-discrete element method (FDEM) to investigate the development of an excavation damaged zone (EDZ) around tunnels in a clay shale formation known as Opalinus Clay. The 3D FDEM was first calibrated against standard laboratory experiments, including Brazilian disc test and uniaxial compression test. The effect of increasing confining pressure on the mechanical response and fracture propagation of the rock was quantified under triaxial compression tests. Polyaxial (or true triaxial) simulations highlighted the effect of the intermediate principal stress (s2) on fracture directions in the model: as the intermediate principal stress increased, fractures tended to align in the direction parallel to the plane defined by the major and intermediate principal stresses. The peak strength was also shown to vary with changing s2.

1. Introduction

Clay shales possess favourable long-term isolation properties, and as a result, have been considered as a possible host rock for the geological disposal of radioactive waste. However, during the excavation, the isolation properties of the intact rock can be degraded as an excavation damaged zone (EDZ) forms around the underground openings. Numerical modelling has been extensively used to understand the failure mechanisms that lead to the formation of an EDZ in Opalinus Clay (a type of clay shale), and in particular, around the tunnel boundaries (e.g. Popp et al., 2008; Yong et al., 2010; Lisjak, 2013; Lisjak et al., 2014a). Among others, these studies have provided valuable insights into the failure processes involved during the formation of EDZ in Opalinus Clay. Nevertheless, these studies were either performed using two-dimensional (2D) methods or simplistic numerical tools.

The present study should be considered the first step of a longer-term research project that aims at using three-dimensional (3D) hybrid finite-discrete element method (FDEM) to investigate the development of the EDZ around tunnels in Opalinus Clay. As an initial stage, the feasibility of using the FDEM tool to model 3D problems was assessed both quantitatively and qualitatively by modelling laboratory experiments in rocks, including Brazilian disc test, uniaxial, triaxial, and polyaxial or true triaxial compression tests. The 3D results were compared with 2D FDEM and experimental observations and data.

Particular emphasis was placed on analysing the influence of the intermediate principal stress s2 on rock fracturing and strength near excavation boundaries. Using a prismatic sample, this simulation reproduced the loading conditions of s1 = 0, s2 ≠ 0, s3 = 0 that exist at the tunnel boundary (Fig. 1a).

It is anticipated that the use of 3D models will improve the quality and reliability of the simulations used to investigate the behaviour of Opalinus Clay during the excavation of tunnels and will allow to better understand how the advancement of the tunnel face influences the shape and extension of the EDZ.

2. Previous modelling work

Rock mechanics laboratory experiments have been extensively modelled using continuum, discontinuum, and hybrid continuum—discontinuum methods in 2D and 3D. A full literature review of these studies requires a dedicated article by itself, and thus, only selected publications are discussed here.

Potyondy and Cundall (2004) used PFC2D and PFC3D to model uniaxial and triaxial (biaxial in 2D) tests. Although acceptable fracture patterns were reported, the stress—strain response did not show any brittle to ductile transition even as the confining pressure was increased to s3 = 70 MPa. More recently, Zhang (2014) used a synthetic rock mass approach within PFC3D (Itasca, 2012) and...
reproduced an appropriate brittle to ductile transition in triaxial and true triaxial tests. However, their results showed an artificial increase of model stiffness (Young’s modulus) as the confining pressure increased. Moreover, the peak strength of the true triaxial tests seemed to always increase as the confinement increased.

Kazerani and Zhao (2010) and Kazerani (2013) used bonded particle modelling (BPM) within UDEC (Itasca, 2013a) to model Brazilian and uniaxial compression tests. Their results illustrated that as the confining pressure increased, more isolated fractures developed and it became more difficult to determine a plane of failure. Also, as the confinement increased so did the material stiffness. In addition, Gao and Stead (2014) used a modified Voronoi method within UDEC and 3DEC (Itasca, 2013a, b) to model laboratory experiments. While their 2D uniaxial model exhibited a shear-dominated failure mechanism, the equivalent 3D model exhibited a more realistic, tensile-dominated mechanism. They attributed this phenomenon to the lack of porosity in the 2D sample, which was effective under a plane strain condition, thus limiting the out-of-plane deformation. Their Brazilian simulation showed a mixture of tensile splitting fractures and shear fractures closer to loading platens.

Jia et al. (2012) used RFPA3D to model polyaxial experiments and tunnel excavations in 3D. They showed that, with the increase of confining pressure, the damaged elements align themselves parallel to the free surface with zero confinement. Scholtès and Donzé (2013) used 3D YADE discrete element method (DEM) code to model laboratory experiments and reproduced acceptable failure envelopes and stress–strain responses, including the brittle–ductile transition with increasing confinement. However, the bond failures did not seem to form any type of macroscopic features (fracture planes).

Pan et al. (2012) used EPCA3D (Pan et al., 2009) to study the influence of intermediate principal stress on rock failure and were able to capture the variation of strength due to $\sigma_2$. They argued that this variation is attributed both to the failure criterion used (Drucker–Prager) which incorporates $\sigma_2$ and to the rock heterogeneity. However, some of the critical inputs to the model were not based on physical quantities that could be assessed experimentally (e.g. plastic strains $\varepsilon^p_2$ and $\varepsilon^p_3$). Moreover, although the failed ‘cells’ were influenced by $\sigma_2$, the fracture angles seemed insensitive to increasing $\sigma_2$.

Elmo (2006) used 2D and 3D ELFEN FDEM code (Rockfield, 2003) to model cylindrical and prismatic uniaxial compression tests. The models did not appear to show a realistic fracturing process and any plane of failure. Cai (2008) used ELFEN to study the influence of intermediate principal stress on the mechanical response of a rock. Their polyaxial simulations were performed under loading conditions similar to this study ($\sigma_1 \neq 0, \sigma_2 \neq 0, \sigma_3 = 0$) and reproduced fractures parallel to maximum and intermediate principal stresses. Due to intrinsic assumptions of ELFEN, Mode II fracturing was not modelled. Also, the fracturing process, including coalescence of individual fractures into fractures planes was not reproduced in their results. More recently, Hamdi et al. (2014) used 3D ELFEN to model Brazilian and compression tests. The Brazilian disc simulations showed reasonable fracturing, while in the uniaxial compression tests it was difficult to distinguish fracture planes. They captured the brittle to ductile transition as the confinement increased. However, the pre-peak stress–strain responses showed a perfectly linear behaviour.

3. Modelling software: FDEM

The hybrid FDEM is a numerical method which combines continuum mechanics principles with DEM algorithms to simulate multiple interacting deformable bodies (Munjiza, 2004). In 3D FDEM, each solid is discretized as a mesh consisting of nodes and tetrahedral elements. An explicit time integration scheme is applied to solve the equations of motion for the discretized system and to update the nodal coordinates at each simulation time step. In general, the governing equation can be expressed as (Munjiza et al., 1995):

$$
M \frac{\partial^2 \mathbf{x}}{\partial t^2} + C \frac{\partial \mathbf{x}}{\partial t} + F_{\text{int}}(\mathbf{x}) - F_{\text{ext}}(\mathbf{x}) - F_c(\mathbf{x}) = 0
$$

where $M$ and $C$ are the system mass and damping diagonal matrices, respectively; $\mathbf{x}$ is the vector of nodal displacements; $F_{\text{int}}$, $F_{\text{ext}}$, and $F_c$ are the vectors of internal resisting forces, applied external loads, and contact forces, respectively.

Contact forces, $F_c$, are calculated either between contacting discrete bodies or along internal discontinuities (i.e. pre-existing or newly created fractures) (Section 3.1). Internal resisting forces, $F_{\text{int}}$, include the contribution from the elastic forces, $F_e$, and the crack element bonding forces, $F_b$, which are used to simulate material elastic deformation and progressive failure, respectively, as further explained in Sections 3.2 and 3.3.

Numerical damping is introduced in the governing equation to account for energy dissipation due to non-linear material behaviour or to model quasi-static phenomena by dynamic relaxation (Munjiza, 2004). The matrix $C$ is equal to
\[ C = \mu I \]

where \( \mu \) and \( I \) are the damping coefficient and the identity matrix, respectively.

3.1. Contact detection and interaction

An FDEM simulation can comprise a very large number of potentially interacting distinct elements. To correctly capture this behaviour, contacting couples (i.e. pairs of contacting discrete elements) must first be detected. Subsequently, the interaction forces, \( F_i \), resulting from such contacts can be defined. Contact interaction forces are calculated between all pairs of elements that overlap in space. Two types of forces are applied to the elements of each contacting pair (i.e. couples) are calculated using a penalty function method (Munjiza, 2004). Contacting couples tend to penetrate into each other, generating distributed contact forces, which depend on the shape and size of the overlap between the two bodies and the value of the penalty term, \( p_\text{pen} \). As penalty values tend to infinity, a body impenetrability condition is approached. The frictional forces between contacting couples are calculated using a Coulomb-type friction law. These frictional forces are used to simulate the shear strength of intact material and of pre-existing and newly created fractures (Mahabadi et al., 2012).

3.2. Elastic behaviour

Since the material strain is expected to be localised in the crack elements (see Section 3.3), the bulk material is treated as linear-elastic using constant-strain tetrahedral elements. Since Opalinus Clay shows strong transverse isotropy, the Hooke’s law based on Young’s modulus and Poisson’s ratio in the x-y symmetry plane \((E_{1}p_{1})\), Young’s modulus and Poison’s ratio in the z-direction \((E_{2}p_{2})\), and shear modulus in z-direction \((G_{2})\) has been implemented in the code (Fig. 1b). The stiffness matrix for transversely isotropic materials is given as (Singh, 2007):

\[
\begin{bmatrix}
\sigma_{xx} & \sigma_{yx} & \sigma_{zz} & \sigma_{zx} & \sigma_{zy} \\
\sigma_{yx} & \frac{1 - \nu_{pz}\nu_{pz}}{E_{p}E_{z}} & \frac{\nu_{p} + \nu_{pz}\nu_{pz}}{E_{p}E_{z}} & \frac{\nu_{p} + \nu_{pz}\nu_{pz}}{E_{p}E_{z}} & 0 \\
\sigma_{zz} & \frac{\nu_{pz} + \nu_{pz}\nu_{pz}}{E_{p}E_{z}} & \frac{1 - \nu_{pz}\nu_{pz}}{E_{p}E_{z}} & \frac{\nu_{p} + \nu_{pz}\nu_{pz}}{E_{p}E_{z}} & 0 \\
\sigma_{zx} & \frac{\nu_{p} + \nu_{pz}\nu_{pz}}{E_{p}E_{z}} & \frac{\nu_{p} + \nu_{pz}\nu_{pz}}{E_{p}E_{z}} & \frac{1 - \nu^{2}_{p}}{E_{p}^{2}E_{z}} & 0 \\
\sigma_{zy} & 0 & 0 & 0 & 0 \\
\sigma_{xy} & 0 & 0 & 0 & 0 \\
\sigma_{yy} & \frac{E_{p}}{1 + \nu_{p}} & 0 & 0 & 0 & 0
\end{bmatrix}
\]

where

\[
\Delta = \frac{(1 + \nu_{p})(1 - \nu_{p} - 2\nu_{pz}\nu_{pz})}{E_{p}^{2}E_{z}}
\]

\[
\nu_{zp} = \frac{E_{z}}{E_{p}}
\]

In general, the elastic response of an FDEM model depends not only on the constitutive relationship of the tetrahedral elements but also on the properties of the crack elements. Since the elastic deformation before the onset of fracturing takes place in the bulk material, no deformation should in theory occur in the crack elements before the intrinsic strength is exceeded. However, a finite stiffness is required for the crack elements by the explicit time integration scheme of FDEM. Such an artificial compliance is represented by the normal, tangential, and fracture penalty values, \( p_n \), \( p_t \), and \( p_f \) for compressive, shear, and tensile loading conditions, respectively. For practical purposes, the contribution of crack elements to the overall model compliance can be largely limited by adopting very high penalty values (Mahabadi et al., 2012). Consequently, the elastic response is effectively controlled by the choice of the stress—strain relationship of the continuum tetrahedral elements.

3.3. Material failure

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 (Dugdale, 1960; Barenblatt, 1962). This approach aims at capturing the non-linear interdependence between stresses and strains that characterises the zone ahead of a macro-crack tip known as the fracture process zone (FPZ). As depicted in Fig. 2, the FPZ in brittle rocks manifests itself in the form of micro-cracking and interlocking related to the presence of micro-scale inhomogeneities (e.g. mineral grains and pre-existing defects or voids) (Labuz et al., 1987). When using cohesive-zone models, the failure of the material progresses based solely on the strength degradation of dedicated interface elements (referred herein to as crack elements) and therefore emerges as a natural outcome of the deformation process without employing any additional macroscopic failure criterion.

In the FDEM code, the bonding stresses transferred by the material are decreasing functions of the displacement discontinuity across the crack elements according to the cohesive laws illustrated in Fig. 3b. These constitutive relationships represent a modified version of the crack model response proposed by Munjiza et al. (1999). Mode I (i.e. opening) and Mode II (i.e. shearing) fracturing are simulated by a cohesive model based on the FPZ model originally developed for concrete by Hillerborg et al. (1976) under the name of fictitious crack model. A Mode I fracture is assumed to initiate when the crack tip opening, \( o_\text{cr} \), reaches a critical value, \( o_\text{cr} \), related to the intrinsic tensile strength of the material, \( f_t \). When the crack opens, the normal bonding stress, \( \sigma \), is not assumed to fall to zero at once but to decrease with increasing crack opening until a residual opening value, \( o_\text{r} \), is reached and a stress-free surface is created (i.e. \( \sigma=0 \)). Mode II (i.e. shearing) fracturing is simulated by a slip-weakening model conceptually similar to that of Ida (1972). For shear loading conditions, a tangential bonding stress, \( \tau \), exists between the two fracture walls, which is a function of the amount of slip, \( s \), and the normal stress on the fracture, \( \sigma_n \). The critical slip, \( s_p \), corresponds to the intrinsic shear strength of the rock, \( f_s \), defined by the Mohr-Coulomb failure criterion as

\[
f_s = c + \sigma_n \tan \phi
\]

where \( c \) is the material cohesion, \( \phi \) is the internal friction angle of the material, and \( \sigma_n \) is the normal stress acting across the fracture surfaces. Upon undergoing the critical slip, \( s_p \), the tangential bonding stress is gradually reduced to a residual value, \( f_r \), which corresponds to a purely frictional resistance:

\[
f_r = \sigma_n \tan \phi
\]
In the current crack element implementation, the unloading path in the softening branch coincides with the loading path. Therefore, the model is strictly valid for monotonic loading conditions only.

For mixed mode fracturing, the rupture of a crack element is defined by the following coupling criterion between crack opening and slip:

\[
\frac{\sigma - \sigma_p}{\sigma_{r} - \sigma_p} > \frac{s - s_p}{s_{r} - s_p} \geq 1
\]  

(8)

The external energy required to fully break a unit surface area of cohesive crack corresponds to the input specific fracture energy, \( G_c \). \( G_c \) is defined in terms of the material properties \( G_{Ic} \) and \( G_{IIc} \) which correspond to the strain energy release rates for Mode I and Mode II fracturing.

Fig. 2. Cohesive-zone approach for material failure modelling in FDEM. (a) Conceptual model of a tensile crack in a heterogeneous rock material (modified after Labuz et al. (1987)). (b) Theoretical FPZ model of Hillerborg et al. (1976). (c) Cross-section of FDEM implementation of the FPZ using tetrahedral elastic elements and six-noded crack elements to represent the bulk material and the fracture, respectively. Triangles are shrunk for illustration purposes.

Fig. 3. Simulation of fracturing with the FDEM code. (a) Representation of a cross-section of a continuum using cohesive crack elements interspersed throughout a mesh of tetrahedral elastic elements. Triangles are shrunk for illustration purposes. (b) Constitutive behaviour of the crack elements defined in terms of normal and tangential bonding stresses, \( \sigma \) and \( \tau \), vs. crack relative displacements, \( o \) and \( s \) (i.e. opening and sliding).
fracturing, respectively. The crack residual displacement values, $o_r$ and $s_r$, are such that:

$$G_{Ic} = G_{IIc} \int_{o_p}^{o_r} \sigma(\alpha) d\alpha$$

$$G_{Ic} = \int_{s_p}^{s_r} \left[ \tau(s) - f_0 \right] ds$$

(9)

Following an approach similar to that pioneered by Xu and Needleman (1996), the crack elements in FDEM are interspersed throughout the material (i.e. across the edges of all tetrahedral element pairs) from the very beginning of the simulation. Thus, cracks are allowed to nucleate and grow without any additional assumption or criterion other than the crack element constitutive response. Upon breakage of the cohesive surface, the crack element is removed from the simulation and therefore the model transition from a continuum to discontinuum is locally completed. The newly created discontinuity is treated by the contact algorithm through the contact forces, $F_c$, briefly described in the previous section. As the simulation progresses, finite displacements and rotations of discrete bodies are allowed and new contacts are automatically recognised.

4. Modelling methodology

4.1. Geometry and boundary conditions

As the model geometries in Fig. 4 show, the 3D laboratory-scale models included a 17.4 mm (diameter) × 35.8 mm (height) cylindrical specimen for the uniaxial and triaxial compression tests, a 29.85 mm (diameter) × 14.85 mm (thickness) circular disc specimen for the Brazilian test, and a prismatic specimen with a square cross-section of 8.7 mm × 8.7 mm and a height of 35.8 mm for the polyaxial (true triaxial) tests. The specimens were meshed with a uniform, unstructured tetrahedral grid of nominal element size of $h = 2.0$ mm (Fig. 4). The top and bottom of the Brazilian disc were flattened over the width of an element to avoid point loading (Fig. 4a). The equation of motion for the discretized system, Eq. (1), was integrated with a time step of $5 \times 10^{-7}$ ms; this value was the largest time step size that ensured numerical stability for the explicit time integration scheme of the code. Uniaxial loading conditions were obtained by means of two rigid platens moving in opposite directions. As shown in Fig. 4d, the loading velocity linearly increased from zero over $t_1 = 30,000$ time steps to a constant value of $v_1 = 1$ m/s. This gradual application of the velocity minimised dynamic artefacts in the system. The FDEM graphical user interface Y-GUI (Mahabadi et al., 2010) was used to assign boundary conditions and material properties to the model.

4.2. Input parameters

As reported in Table 1, input parameters were based on material properties previously calibrated by Lisjak et al. (2014b). Since the current 3D formulation does not account for strength anisotropy, the calibrated strength parameters were averaged and used as inputs for the 3D simulations (Table 1). A friction coefficient equal to 0.1 was assumed at the platen-sample interfaces. The effect of the crack element compliance on the overall model stiffness was minimised by selecting appropriate values for the penalty coefficients. Based on the recommendations of Mahabadi et al. (2012), normal penalty, $p_n$, tangential penalty, $p_t$, and fracture penalty, $p_f$, were set equal to 10, 10, and 5 times of the average Young's modulus, $E$, respectively. As illustrated in Fig. 1b, the $x$-$y$ plane is assumed to be the plane of symmetry for the transversely isotropic constitutive law of Eq. (3), representing the P-sample of Lisjak (2013).

5. Results

In this section, the results of the Brazilian disc test, unconfined uniaxial compression test, the triaxial and polyaxial (true triaxial) compression tests at different confining pressures are discussed. Note that throughout this manuscript, compressive stresses are negative.

5.1. Brazilian disc test

The stress evolution ($\sigma_{zz}$) and fracturing process of the Brazilian disc are illustrated in Fig. 5. As the specimen is loaded, tensile stresses form in the centre of the disc. However, high shear stresses also develop closer to the loading platens. Thus, the specimen experiences a mix of tensile failure along the loading direction and crushing failure closer to the loading points. Similar trends in 3D simulations have been reported by other researchers (Gao and Stead, 2014).

Fig. 4. 3D meshes of (a) the Brazilian disc test, (b) uniaxial and triaxial compression tests, and (c) polyaxial tests. (d) Loading was applied by prescribed velocities ($v$) that followed a linear increase to $v_1$ over $t_1$ time steps. Dimensions are given in units of millimetres.
It is argued that tensile failure would dominate over shear failure if a lower Mode I fracture energy ($G_{Ic}$) was used (Table 1). This phenomenon is clearly demonstrated when the value was reduced to $G_{Ic} = 0.02$ J/m$^2$ (Fig. 6). Note that $G_{Ic}$ is related to Mode I fracture toughness ($K_{Ic}$) through Young’s modulus. However, if $K_{Ic}$ is not available, $G_{Ic}$ should be calibrated via an iterative process as depicted by Tatone (2014).

The indirect tensile strength of the Brazilian disc, calculated as

$$
\sigma_t = \frac{2P}{\pi DB}
$$

is shown in Fig. 7 (with $P$ as the reaction force, $D$ as the disc diameter, and $B$ as the disc thickness). As expected, the stresses increased linearly until reaching about 80% of the peak (strain hardening), where the linearity was lost. Upon reaching the peak stress, brittle failure was followed during which the stresses decreased in the post-peak (strain softening). The tensile strength was slightly overestimated compared to the laboratory experiments with a tensile strength ranging between 0.67 MPa and 1.5 MPa.

5.2. Uniaxial and triaxial compression tests

Triaxial simulations were performed using variable $\sigma_3$ values of 1 MPa, 2.5 MPa, 5 MPa, 7.5 MPa, 10 MPa, and 12.5 MPa. Similar to the loading velocity, the confining pressure was applied gradually over 30,000 time steps (Fig. 4d).

5.2.1. Fracturing process

Fig. 8 demonstrates the major principal stress ($\sigma_1$) and the fracture pattern of the uniaxial specimen along two orthogonal

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**Table 1**

Input parameters of the FDEM model calibrated based on laboratory-scale rock mechanics tests on Opalinus Clay (Lisjak et al., 2014b).

<table>
<thead>
<tr>
<th>Continuum tetrahedral elements</th>
<th>Crack elements</th>
<th>Numerical parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bulk density, $\rho$ (kg/m$^3$)</td>
<td>Tensile strength, $f_t$ (MPa)</td>
<td>Viscous damping coefficient, $\mu$ (kg/(m s))</td>
</tr>
<tr>
<td>$2330$</td>
<td>$0.41$</td>
<td>$1.2 \times 10^7$</td>
</tr>
<tr>
<td>Young’s modulus parallel to bedding, $E_p$ (GPa)</td>
<td>Cohesion, $c$ (MPa)</td>
<td>Normal contact penalty, $p_n$ (GPa m)</td>
</tr>
<tr>
<td>$3.8$</td>
<td>$5$</td>
<td>$25.5$</td>
</tr>
<tr>
<td>Young’s modulus perpendicular to bedding, $E_z$ (GPa)</td>
<td>Mode I fracture energy, $G_{Ic}$ (J/m$^2$)</td>
<td>Tangential contact penalty, $p_t$ (GPa/m)</td>
</tr>
<tr>
<td>$1.3$</td>
<td>$3$</td>
<td>$25.5$</td>
</tr>
<tr>
<td>Poisson’s ratio parallel to bedding, $\nu_p$</td>
<td>Mode II fracture energy, $G_{IIc}$ (J/m$^2$)</td>
<td>Fracture penalty, $p_f$ (GPa)</td>
</tr>
<tr>
<td>$0.25$</td>
<td>$22.5$</td>
<td>$12.5$</td>
</tr>
<tr>
<td>Poisson’s ratio perpendicular to bedding, $\nu_{zp}$</td>
<td>Friction angle of intact material, $\phi_i$ (°)</td>
<td></td>
</tr>
<tr>
<td>$0.35$</td>
<td>$22$</td>
<td></td>
</tr>
<tr>
<td>Shear modulus, $G_{st}$ (GPa)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$0.9$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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Fig. 5. Stress ($\sigma_{zz}$) and the fracture pattern of the Brazilian specimen along $y$-$z$ plane during the simulation time at (a) 0.05 ms, (b) 0.1 ms, (c) 0.15 ms, (d) 0.2 ms, (e) 0.25 ms, and (f) 0.3 ms after the start of simulation, respectively. Compressive stresses are negative. The bottom right inset shows where the cross-sections were taken.
views (x-y and y-z planes) during the simulation time. As the specimen was gradually loaded (Fig. 8a–d), isolated fractures formed in various locations in the specimen (Fig. 8e–h). These fractures later coalesced to form more macroscopic fractures (Fig. 8i–l). Fracturing of the triaxial specimen at $\sigma_3 = 1$ MPa followed a similar trend as the uniaxial model.

X-ray style 3D fracture volume evolution of the specimen during the simulation time is presented in Fig. 9. The gray-scale intensity in these images represents fractures localised into planes, i.e. fracture density. As shown in Fig. 9d, the major planes of failure were aligned approximately at 52° from the x-z plane. This value corresponds well with the theoretical value according to the Mohr-Coulomb criterion: $\pi/4 + \phi/2 = 56°$.

The application of more confining pressure ($\sigma_3 \geq 2.5$ MPa) limited the growth of tensile fractures parallel to the major principal stress direction (parallel to y-axis), thus resulting in a more shear-dominated fracturing process. Unlike the models at low confinement ($\sigma_3 = 0–1$ MPa), in which one or two major macroscopic fractures developed, the fractures in triaxial models with $\sigma_3 \geq 2.5$ MPa formed shear bands or faults (Figs. 10 and 11). As the confining pressure exceeded 5 MPa, in fact, the case of $\sigma_3 = 12.5$ MPa in Figs. 12 and 13, shear failures formed a network of small fractures that continued to deform plastically. As a result, no noticeable plane of failure was formed and a more ductile post-yield stress response was captured (see Section 5.2.2). These types of fracturing behaviour correspond well with the published literature of experimental observations (Mogi, 2007; Mahabadi, 2012) and of previous 2D FDEM simulations (Mahabadi, 2012; Lisjak et al., 2014b).

5.2.2. Mechanical response

The stress–strain curves of the uniaxial and triaxial simulations are presented in Fig. 14 (major principal stress, $\sigma_1$, vs. major principal strain, $\varepsilon_1$). At low or no confining pressure ($\sigma_3 = 0–2.5$ MPa), the specimen showed strain hardening until reaching the peak strength, which was then followed by brittle strain softening, during which the stresses decreased rapidly. As the confining pressure increased, the peak strength increased and a more ductile post-peak behaviour was observed ($\sigma_3 = 5$ MPa). At higher confining pressures ($\sigma_3 > 5$ MPa), a completely ductile post-peak was simulated. Overall, this trend agrees with laboratory findings and previous numerical simulations performed in 2D (Lisjak et al., 2014b). It should be noted that the strains in Fig. 14 were calculated from platen displacements divided by specimen height.

The stress–strain curves seemed to depart from linearity at about 60%–70% of peak stress (Fig. 14). This range coincides with the so-called crack damage stress, which marks the beginning of unstable cracking (Bieniawski, 1967; Martin and Chandler, 1994). In the case of an FDEM simulation, this stage is represented by softening of individual crack elements.

Fracturing in rocks usually occurs parallel to the major principal stress ($\sigma_1$) direction. Therefore, applying any confining pressure tends to arrest the initiation and development of fractures. For this reason, the rock exhibits higher strength, possibly strain hardening, and less fracturing occurs as the confining pressure increases.

For comparison, 2D uniaxial and biaxial models were built using similar element sizes and loading rates as the 3D models (Fig. 15). Unlike the 3D models, the 2D models showed a perfectly linear elastic mechanical response up until yielding, followed by a sudden drop in the post-peak stress at low confining pressures ($\sigma_3 = 0–5$ MPa) or by strain hardening at higher pressures ($\sigma_3 \geq 7.5$ MPa). Both the 2D and 3D models captured the increase in strength as the confinement increased.

Using the results of the Brazilian, uniaxial, and triaxial (biaxial in 2D) tests, the failure envelope of the simulations was derived (Fig. 16). While both the 3D and 2D failure envelopes reproduced the increase in peak strength as a function of increasing confining pressure, the 3D envelope significantly underestimated the slope of the curve, which corresponds to the emergent internal friction angle (Table 2). However, the simulated cohesion was relatively close to the input value. Since the model inputs, in particular, penalty terms were adopted from calibrated 2D simulations, further investigation is required to assess the validity of these parameters in 3D.
Fig. 8. Major principal stress ($\sigma_1$) and the fracture pattern of the uniaxial specimen along two orthogonal views (x-y and y-z planes) during the simulation time at (a) 0 ms, (b) 0.0625 ms, (c) 0.125 ms, (d) 0.1875 ms, (e) 0.199 ms, (f) 0.2015 ms, (g) 0.2065 ms, (h) 0.2115 ms, (i) 0.2165 ms, (j) 0.2215 ms, (k) 0.2265 ms, and (l) 0.2315 ms after the start of simulation, respectively. Compressive stresses are negative.

Fig. 9. 3D fracture volume of the uniaxial specimen during the simulation time at (a) 0.2015 ms, (b) 0.2115 ms, (c) 0.2215 ms, and (d) 0.2315 ms after the start of simulation, respectively. The dashed lines in (d) represent approximate failure plane orientations.
Finally, the 3D models captured the elastic response of the material very well: the emergent Young’s modulus showed a merely 5% divergence from the input value (Table 2).

5.3. Polyaxial compression tests

Polyaxial or true triaxial simulations were performed using $\sigma_3 = 0$ MPa with variable $\sigma_2$ values of 0 MPa, 1 MPa, 2.5 MPa, 5 MPa, 7.5 MPa, 10 MPa, and 12.5 MPa. Initial simulation runs revealed that the models with $\sigma_2 = 10–12.5$ MPa would fracture mainly due to the rapid application of $\sigma_2$. Therefore, unlike the triaxial models where the confining pressure was applied gradually over 30,000 time steps (Fig. 4d), the intermediate principal stress in the polyaxial models was applied gradually at a rate of 80 MPa/ms until reaching the prescribed, constant value.

5.3.1. Fracturing process

The fracture propagation of the polyaxial model with $\sigma_2 = 0$ MPa is demonstrated in Figs. 17 and 18. Similar to the uniaxial and triaxial models (Figs. 8 and 9), the formation of two distinct fracture planes parallel to $\sigma_2$ can be observed. A similar behaviour was noticed for $\sigma_2 = 1$ MPa and 2.5 MPa.

As the intermediate principal stress increased, $\sigma_2 \geq 5$ MPa, the angle between the faults and the maximum principal stress $\sigma_1$, direction was significantly reduced (Figs. 19 and 20). As a result, two distinct fracture planes can be easily distinguished in Fig. 20 where the fractures are parallel to $\sigma_2$ and are mainly in the direction of $\sigma_1$. This finding agrees with experimental observations (Mogi, 1967). Also, this kind of fracturing is similar to spalling-type fractures observed around underground openings. Similar to the triaxial simulations, at higher intermediate principal stresses ($\sigma_2 = 10–12.5$ MPa), more isolated fractures formed and it became harder to distinguish well-defined fracture surfaces (Figs. 21 and 22).

5.3.2. Mechanical response

The stress–strain response of the polyaxial models and the peak maximum principal stress versus the intermediate principal stress ($\sigma_1$ vs. $\sigma_2$) are presented in Fig. 23. The addition of $\sigma_2$ initially
Fig. 11. 3D fracture volume of the triaxial specimen with $\sigma_3 = 5$ MPa during the simulation time at (a) 0.2505 ms, (b) 0.2805 ms, (c) 0.3105 ms, and (d) 0.3375 ms after the start of simulation, respectively.

Fig. 12. Major principal stress ($\sigma_1$) and the fracture pattern of the triaxial specimen with $\sigma_3 = 12.5$ MPa along two orthogonal views (x-y and y-z planes) during the simulation time at (a) 0 ms, (b) 0.125 ms, (c) 0.25 ms, (d) 0.2925 ms, (e) 0.3175 ms, (f) 0.3425 ms, (g) 0.3675 ms, (h) 0.3925 ms, (i) 0.4175 ms, (j) 0.4425 ms, (k) 0.4675 ms, and (l) 0.4925 ms after the start of simulation, respectively. Compressive stresses are negative.
increased the peak stress ($\sigma_1$), reaching the peak increase at $\sigma_2 = 5$ MPa. In contrast, at higher $\sigma_2$ values ($\sigma_2/C_2 > 7.5$), $\sigma_1$ decreased (Fig. 23 right). The $\sigma_1$-$\sigma_2$ relationship showed a downward concave shape. This general trend is in good agreement with published experimental results (Mogi, 1967; Haimson and Chang, 2000; Haimson, 2006; Colmenares and Zoback, 2002; Paterson and Wong, 2005; Chang and Haimson, 2012) and rock failure criteria that incorporate $\sigma_2$ (Wiebols and Cook, 1968; Benz and Schwab, 2008).

![Fig. 13. 3D fracture volume of the triaxial specimen with $\sigma_3 = 12.5$ MPa during the simulation time at (a) 0.3175 ms, (b) 0.3675 ms, (c) 0.4175 ms, and (d) 0.4675 ms after the start of simulation, respectively.](image)

![Fig. 14. Stress–strain curves of the 3D uniaxial and triaxial compression test simulations.](image)

![Fig. 15. Stress–strain curves of the 2D uniaxial and biaxial compression test simulations.](image)

![Fig. 16. Failure envelope of the 3D Brazilian, uniaxial, and triaxial compression simulations for 3D and 2D simulations (Lisjak et al., 2014b) and experiments (Popp et al., 2008; NAGRA, 2008). Error bars correspond to standard deviation of the laboratory experiments.](image)

![Table 2](image)

<table>
<thead>
<tr>
<th>Case</th>
<th>Young’s modulus parallel to bedding, $E_p$ (GPa)</th>
<th>Cohesion, $c$ (MPa)</th>
<th>Friction angle of intact material, $\phi_i$ (°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3D</td>
<td>3.6 ($-5%$)</td>
<td>6.09 (22%)</td>
<td>12.2 ($-45%$)</td>
</tr>
<tr>
<td>2D</td>
<td>3.3 ($-13%$)</td>
<td>4.06 ($-19%$)</td>
<td>26.6 (21%)</td>
</tr>
<tr>
<td>Experiment</td>
<td>3.8</td>
<td>5.00</td>
<td>22.0</td>
</tr>
</tbody>
</table>
Nonetheless, comparison with literature indicates that the extent of the change may be underestimated by the code (similar to the triaxial models). Using another FDEM code, Cai (2008) also underestimated the influence of the intermediate principal stress. Mogi (1967, 1971) among others showed that the increase of peak stress is more pronounced at higher $\sigma_3$ values and for brittle rather than ductile material. Therefore, to further study the effect of $\sigma_2$ on peak strength, various values of $\sigma_3$ should be used (versus $\sigma_3 = 0$).

Fig. 17. Major principal stress ($\sigma_1$) and the fracture pattern of the polyaxial specimen with $\sigma_2 = 0$ MPa along two orthogonal views during the simulation time at (a) 0 ms, (b) 0.05 ms, (c) 0.1 ms, (d) 0.15 ms, (e) 0.18 ms, (f) 0.19 ms, (g) 0.2 ms, (h) 0.21 ms, (i) 0.2185 ms, (j) 0.227 ms, (k) 0.2355 ms, and (l) 0.244 ms after the start of simulation, respectively. Compressive stresses are negative.

Fig. 18. 3D fracture volume of the polyaxial specimen with $\sigma_2 = 0$ MPa during the simulation time at (a) 0.2 ms, (b) 0.21 ms, (c) 0.227 ms, and (d) 0.244 ms after the start of simulation, respectively.
MPa used in this work). However, this was outside the scope of the current study.

Since the Mohr-Coulomb failure criterion, which is used in our FDEM code, ignores the effect of the intermediate principal stress, the peak strength should be insensitive to $\sigma_2$. However, the code successfully captured the dependence of peak $\sigma_1$ on $\sigma_2$, albeit to a lower degree, as an emergent property, meaning that this behaviour was not a result of the constitutive relationships implemented in the model but an emerging property of the simulations. Regardless, to capture the influence of the intermediate principal stress in full, a failure criterion that incorporates $\sigma_2$ in its formulation should be used (e.g. Drucker–Prager, Wiebols and Cook, or modified Mohr-Coulomb formulations considering $\sigma_2$ (Singh et al., 2011)). Pan et al. (2012) argued that, if using Mohr-

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Fig. 19. Major principal stress ($\sigma_1$) and the fracture pattern of the polyaxial specimen with $\sigma_2 = 5$ MPa along two orthogonal views during the simulation time at (a) 0.0625 ms, (b) 0.125 ms, (c) 0.174 ms, (d) 0.1865 ms, (e) 0.199 ms, (f) 0.2115 ms, (g) 0.224 ms, (h) 0.2365 ms, (i) 0.249 ms, (j) 0.2615 ms, (k) 0.274 ms, and (l) 0.2865 ms after the start of simulation, respectively. Compressive stresses are negative.

Fig. 20. 3D fracture volume of the polyaxial specimen with $\sigma_2 = 5$ MPa during the simulation time at (a) 0.1865 ms, (b) 0.2115 ms, (c) 0.2365 ms, and (d) 0.2865 ms after the start of simulation, respectively.
Coulomb, $\sigma_2$ dependence is also related to rock heterogeneity. However, their heterogeneous simulations using Mohr-Coulomb still underestimated $\sigma_2$ dependence compared with simulations using Drucker-Prager criterion.

Peculiarly, the specimens with $\sigma_2 = 10-12.5$ MPa showed a higher stiffness (Fig. 23). The reason for this artefact remains unclear and requires further research.

6. Concluding remarks

The 3D FDEM was used to study the mechanical response and damage evolution of Opalinus Clay during classic laboratory tests. To better reproduce the response of the rock, a transversely isotropic formulation for elastic deformation was incorporated in the code.

The Brazilian disc simulation showed reasonable fracture trajectories, while the tensile strength was slightly larger than the range of experimental values. The uniaxial tests showed a realistic fracturing process with fractures coalescing into noticeable fracture planes. The effect of increasing confining pressure was captured in both the brittle-ductile transition of the stress-strain response and fracture patterns. Similar to the 2D simulations (Lisjak et al., 2014b), the failure envelope of the 3D simulations tended to be in the lower range of the experimental values as the confining pressure increased. However, unlike the 2D simulations, the 3D results

Fig. 21. Major principal stress ($\sigma_1$) and the fracture pattern of the polyaxial specimen with $\sigma_2 = 10$ MPa along two orthogonal views during the simulation time at (a) 0.075 ms, (b) 0.1 ms, (c) 0.125 ms, (d) 0.15 ms, (e) 0.175 ms, (f) 0.2 ms, (g) 0.225 ms, and (h) 0.25 ms after the start of simulation, respectively. Compressive stresses are negative.

Fig. 22. 3D fracture volume of the polyaxial specimen with $\sigma_2 = 10$ MPa during the simulation time at (a) 0.175 ms, (b) 0.2 ms, (c) 0.225 ms, and (d) 0.25 ms after the start of simulation, respectively.
underestimated the friction angle of the rock. The choice of numerical parameters requires a comprehensive calibration study. The polyaxial (true triaxial) simulations successfully illustrated the influence of the intermediate principal stress ($\sigma_2$) on the fracturing process of the rock. It was shown that the major planes of failure will be parallel to the $\sigma_2$ direction. An increase in $\sigma_2$ values would align the fractures more parallel to the $\sigma_1$ direction, which can be related to spalling-type failure on tunnel sidewalls. The polyaxial results also exhibited the dependence of the peak strength on increasing $\sigma_2$, following a downward concave shape where the peak increase was observed at $\sigma_2 = 5$ MPa. Further investigation, in particular using various $\sigma_3$ values, is required to study this effect. Overall, the 3D simulations presented promising results for the use of 3D FDEM in modelling the mechanical response and damage evolution of the rock.

**Conflict of interest**

The authors wish to confirm that there are no known conflicts of interest associated with this publication and there has been no significant financial support for this work that could have influenced its outcome.

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Fig. 23. Stress–strain curves of the 3D polyaxial compression test simulations.