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

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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 (σ_2) 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 σ_2.

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,σ_2, on rock fracturing and strength near excavation boundaries. Using a prismatic sample, this simulation reproduced the loading conditions of $\sigma_1 \neq 0$, $\sigma_2 \neq 0$, $\sigma_3 = 0$ 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 $\sigma_3 = 70$ MPa. More recently, Zhang (2014) used a synthetic rock mass approach within PFC3D (Itasca, 2012) and

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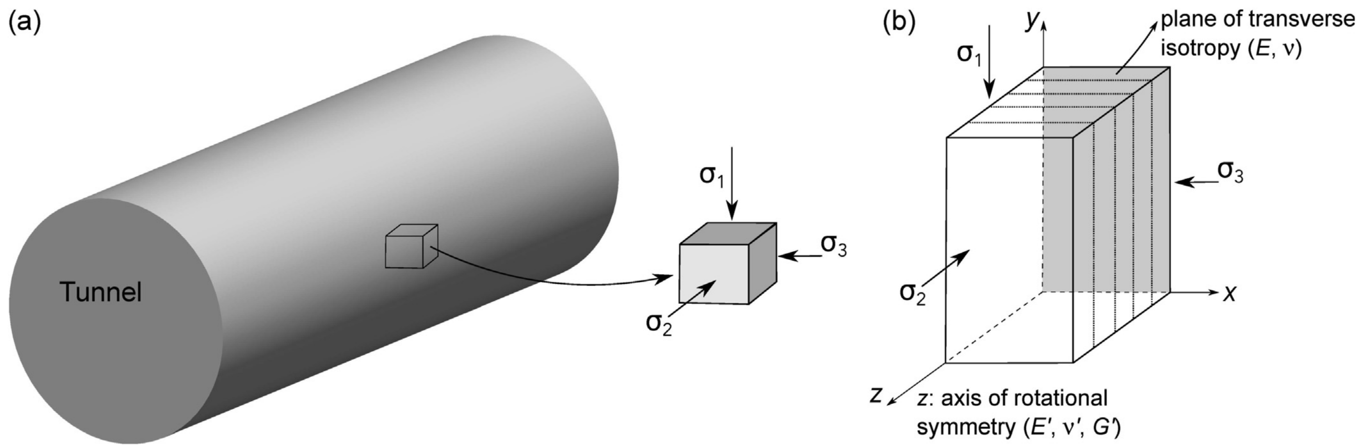

Fig. 1. (a) Schematic of principal stresses around a tunnel. (b) Representation of the transversely isotropic constitutive law.

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 σ_2. They argued that this variation is attributed both to the failure criterion used (Drucker–Prager) which incorporates σ_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 ε_c^p and ε_f^p). Moreover, although the failed 'cells' were influenced by σ_2, the fracture angles seemed insensitive to increasing σ_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):

$$\boldsymbol{M}\frac{\partial^2 \boldsymbol{x}}{\partial t^2} + \boldsymbol{C}\frac{\partial \boldsymbol{x}}{\partial t} + \boldsymbol{F}_{\text{int}}(\boldsymbol{x}) - \boldsymbol{F}_{\text{ext}}(\boldsymbol{x}) - \boldsymbol{F}_{\text{c}}(\boldsymbol{x}) = 0 \tag{1}$$

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

Contact forces, $\boldsymbol{F}_{\text{c}}$, 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, $\boldsymbol{F}_{\text{int}}$, include the contribution from the elastic forces, $\boldsymbol{F}_{\text{e}}$, and the crack element bonding forces, $\boldsymbol{F}_{\text{b}}$, 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 $\boldsymbol{C}$ is equal to