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## Multi-disciplinary characterization of shrinkage effects in Opalinus clay

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Due to its low hydraulic permeability and several beneficial mechanical properties, Opalinus Clay formation (OPA) is considered as a potential host rock for high-level radioactive waste disposal. However, several factors during the excavation and operational stages can endanger the long-term safety of the repositories. One of the major safety concerns in the underground geological repositories includes the formation of shrinkage-induced cracks [1]. Shrinkage-induced cracks, i.e., desiccation cracks, are a result of the underground opening being exposed to lower relative humidity (RH) levels during seasonal changes and subsequent shrinkage deformation. Over the last two decades, OPA has been extensively investigated by several in-situ experiments conducted at the Mont Terri Underground Rock Laboratory (URL) in Switzerland [2]. In particular, the recently established cyclic deformation (CD-A) experiment is aimed at the investigation of the coupled hydro-mechanical processes in the sandy facies of OPA due to the seasonal changes and variations in RH [3]. In this study, to further investigate the mechanical parameters of OPA under various climatic conditions and to capture potential desiccation cracking scenarios, a multi-disciplinary approach, including experimental analysis and numerical simulation, has been adopted. In this regard, the required samples for laboratory tests were taken from drilled cores near the CD-A experiment. Additionally, the observations in CD-A regarding the onset and propagation of desiccation fracturing were used as validation point for verification of the employed numerical method.

In order to characterize the RH-dependent mechanical parameters of the OPA, a customized desiccator cell has been configured and set up at the geomechanics and geotechnics laboratory of CAU. The concept of a humidity-controlled rock laboratory test setup originates from [4]. The experimental setup, as well as its schematic representation, is shown in Figure 1(a). The components of the customized desiccator cell can be divided into four parts, including an isolated epoxy glass cell equipped with RH and temperature sensors, a loading apparatus, a salt bath and a micro-camera tube. The experimental layout contains two distinct stages, namely the equilibrium and loading stages. During the first stage and prior to the onset of mechanical loading, the sample is placed inside the cell, where it is allowed to equilibrate with a certain level of RH. Based on the initial water content of the sample and RH in the cell, the equilibrium stage can last 7-10 days. The RH inside the cell, covering the range between 0.19 and 0.88, was achieved and maintained by employing various saturated salt solutions. In this study, the above-mentioned methodology is employed to investigate the strength characteristics of the OPA under different humidity conditions. For such a purpose, a series of semi-circular threepoint bending experiments (SCB) has been conducted. Furthermore, given the relative angle between the loading direction and plane of isotropy, denoted as  $\theta$ , three types of samples with  $\theta = 0, 45$  and 90° were considered to account for the anisotropic effects. The experimental observations in terms of peak loads obtained during the loading stage against the varying RH in the cell are illustrated in Figure 1(b). In addition to the general decreasing trend for material toughness as a result of increasing RH, the remarkable effect of structural anisotropy on material strength can be seen. It should be noted that, the observed deviation from the overall trend for peak load response of certain samples can be attributed to the generation of the micro-defects in samples during the preparation or the drilling processes, which can lead to alterations in the mechanical properties of the samples.



Figure 1: (a) Customized desiccator cell and its schematic representation, (b) obtained peak loads during semi-circular three-point bending test under different relative humidity conditions. ( $\theta$  refers to relative angle between the loading direction and plane of isotropy in Opalinus clay samples.

To further investigate the shrinkage effects and mechanisms of desiccation fracturing observed in OPA during experimental and field analyses, we utilized and extended the Finite Discrete Element Method (FDEM). In this regard, a hydro-mechanically coupled framework based on the principles of Richards Mechanics is developed to account for the flow in the variably saturated porous medium. The FDEM was originally developed by Munjiza et al. [5]. By combining the principles of the Discrete Element Method (DEM) and Finite Element (FE) analysis, the FDEM is capable of capturing the transition from a continuous to a discontinuous state through the simulation of fracturing and fragmentation processes [6]. To realize the anisotropic mechanical response in OPA, a transversely isotropic stress-strain constitutive law was implemented. Additionally, a strength criterion for each cohesive element was considered based on its relative angle with the macroscopic bedding direction [7].

In order to consider the variably saturated porous media flow within the framework of FDEM, a vertex-centered finite volume scheme is adopted. Based on this approach, a dual grid of polygonal control volumes is subjected to the conservation of the fluid phase. The adopted mass balance equation of water can be expressed as follows

$$S_{w}\alpha \frac{\partial \boldsymbol{\epsilon}_{v}}{\partial t} - n\left(\frac{S_{w}}{K_{w}} - \frac{\partial S_{w}}{\partial p_{w}}\right)\frac{\partial p_{w}}{\partial t} + \nabla \boldsymbol{\cdot} \boldsymbol{q} = 0$$
Eq.1

where  $S_w$  and  $p_w$  are the saturation and pore water pressure, respectively.  $\alpha$  is the Biot's coefficient, *n* is the porosity and  $K_w$  is the water bulk modulus. In Eq. 1,  $\nabla$ . *q* denotes the fluid flux vector. The flow rate vector, *q*, is evaluated based on the unsaturated Darcy flow law. The Van Genuchten constitutive law was used for the definition of the hydraulic behavior in an unsaturated porous medium where the permeability tensor and saturation state are functions of pressure head [8]. The hydro-mechanical coupling was realized based on the principle of effective stress and achieved by adopting a staggered coupling scheme. The methodology was verified against the available benchmarks in the literature. To capture the desiccation cracking in field scale, a model consisting of a 2D cross section of the CD-A experiment was also considered. The required material properties for the numerical model were obtained from experimental results. In complete agreement with field observation in the CD-A experiment, the desiccation cracks start to develop around the underground opening at RH between 97~98%.

This paper presented a multi-disciplinary approach for the characterization of the shrinkage effects in OPA. In this regard, a combination of experimental analysis and numerical modelling techniques has been employed. The experimental work provided a better understanding of the anisotropic mechanical properties of OPA under different humidity conditions. The developed coupled formulation in the FDEM framework has proven to be successful in capturing desiccation fracturing mechanisms in the field scale. The presented methodology would facilitate further investigation of scenarios in which desiccation fracturing is involved.

## **Contributor statement**

Nima Haghighat: Investigation, Methodology, Writing – Original Draft. Amir Shoarian Sattari: Writing – Review & Editing Frank Wuttke: Supervision.

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