ALERT Geomaterials

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POSTER SESSION

Booklet of abstracts

Editor: Nadia Benahmed

(IRSTEA, Aix-en-Provence – France)

ALERT Geomaterials

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Poster Session

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Dear colleagues,

We are pleased to welcome you to Aussois and our 27th ALERT Workshop and School.

As always, it is an exciting time for us to continue to meet and bring together inspired people for fruitful days with interesting, stimulating discussions, exchange of knowledge and experience on Geomechanics. Presentation of recent advances offers the chance to get up-to-date and to remain at the cutting edge.

We would like to express our thanks to all of you who came to Aussois to present and share your own work!

We wish you a good workshop and school experience and a pleasant stay in Aussois!

Kind regards,

Nadia Benahmed.

Table of contents

Constitutive modelling of saturated frozen soil

S. A. Ghoreishian Amiri, G. Grimstad, M. Kadivar
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Keywords: Frozen soil, Constitutive model, Rate effect, Cryogenic suction, Solid-phase stress

Abstract

The mechanical behavior of frozen soils is one of the challenging topics in the field of geotechnical engineering. The behavior of frozen soils is strongly affected by the amount of ice, while on the other hand, the amount of ice depends on the temperature and the applied mechanical stresses. Considering the highly rate dependent behavior of ice, rate sensitive behavior of frozen soils is expected.

The influence of ice content and temperature on the mechanical behavior, the coupling effects on the reverse direction and the highly rate dependent behavior can be mentioned as the main differences between the behavior of frozen and unfrozen soils. In the light of these differences, a constitutive model for describing the stress-strain behavior of saturated frozen soils is proposed. By dividing the total stress into fluid pressure and solid phase stress, in addition to consideration of the cryogenic suction, the model is formulated within the framework of two-stress state variables. The solid phase stress is defined as the combined stress in the soil grains and ice.

The rate dependent behavior is considered by using the so called over-stress method. In this model, elastic-viscoplastic behavior is considered for the deformation due to variation of solid phase stress, while elastic-plastic behavior is assumed for the suction induced deformation. Figure 1 shows the reference, dynamic and yield surfaces of the model.

The proposed model is consistent with the micromechanical description of the behavior due to variation of ice content and temperature; i.e. curvature-induced premelting and interfacial premelting mechanisms (figure 2). The former is the result of surface tension and acts very similar to the capillary suction by bonding the grains together. Whereas the latter is the result of disjoining pressure (as a repelling force between ice and solid grains) and tends to widen the gap by sucking in more water.

The proposed model is able to represent many of fundamental features of the behavior of frozen soils such as ice segregation phenomenon and strength weakening due to pressure melting. In unfrozen state the model becomes a conventional critical state model.

In order to examine the ability of the model to simulate the behavior of frozen soils in an acceptable way, four different series of tests are simulated and compared with model predictions. In the first and second sets, triaxial compression tests on frozen sand samples at different temperatures and confining pressures are simulated to show the ability of the model for representing the behavior with a single set of parameters. In the third one, uniaxial

compression tests on Fairbanks silt at different strain rates are used to show the ability of the model for considering the rate effect. At the end, a set of creep tests on frozen sands at different temperatures and stress levels are simulated and compared with experiments. In addition, some typical predictions of the model for simulating the characteristic trends of the frozen soil behavior is described qualitatively.

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Figures

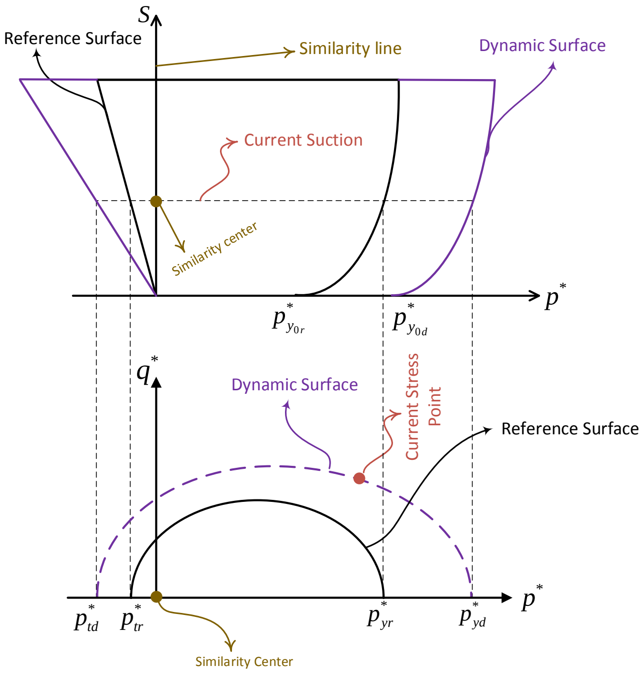

Figure 1 : *Representation of reference, dynamic and yield surfaces*

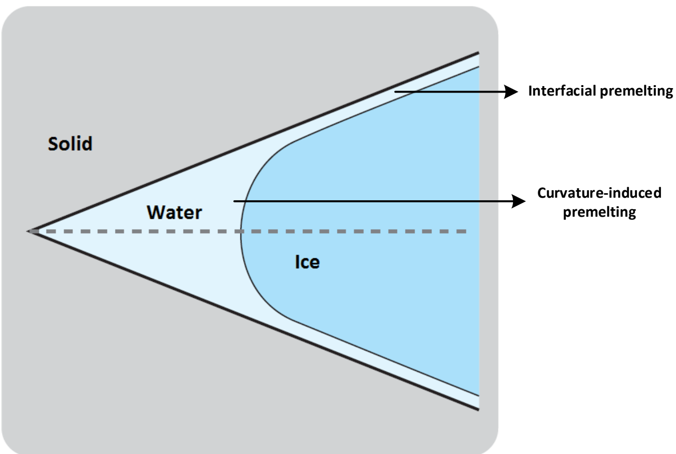

Figure 2 : *Curvature induced premelting and interfacial premelting during intrusion of ice into a wedge-shape wet preferential solid (Zhou, 2014)*

Influence of hydration temperature on the C-S-H structure in an oil well cement paste

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Keywords: Cement paste, C-S-H density, Chemical composition

Abstract

The hydration temperature has a noticeable influence on the mechanical behavior of cement pastes and the related micro and nanostructure. The knowledge of the effect of the curing temperature on the microstructure and mechanical behavior of cement paste is essential for a better understanding of the behavior of the cement sheath in oil wells. Actually, cement sheaths are hydrated under different temperature conditions due to geothermal gradient, which induces significant changes on their microstructure and alter their mechanical properties. This work is an investigation of the curing temperature effect on the microstructure of cement pastes. Cement pastes cured at temperatures, between 7°C and 90°C, were examined using a combination of various experimental techniques: X-Ray diffraction and Rietveld analysis, thermo-gravimetric analysis, mercury intrusion porosimetry, total porosity measurement. The analysis of the results of XRD-Rietveld, TGA experiments and measurement porosity permitted the evaluation of molar C/S and H/S (Saturated) ratios for different temperatures, showing a decrease of these molar ratios with hydration temperature and confirming the enhanced polymerization rate of silicate chain with temperature. The experimental results of porosity measurement show an increase of the capillary porosity with hydration temperature, while the total porosity remains almost constant. This reflects that the gel porosity is decreasing with temperature. The C-S-H density has been evaluated in an analysis combining the results of the above-mentioned experiments. The results show an increase of C-S-H density and a reduction of its internal porosity with increasing hydration temperature. This increase in density explains the observed increase of the capillary porosity and the resulted decrease of the mechanical properties observed at higher hydration temperatures. The reduction of the C-S-H internal porosity highlighted that the densification of the C-S-H is mainly due to changes of the porous structure regardless of the eventual variation of C-S-H solid density with temperature.

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Figures

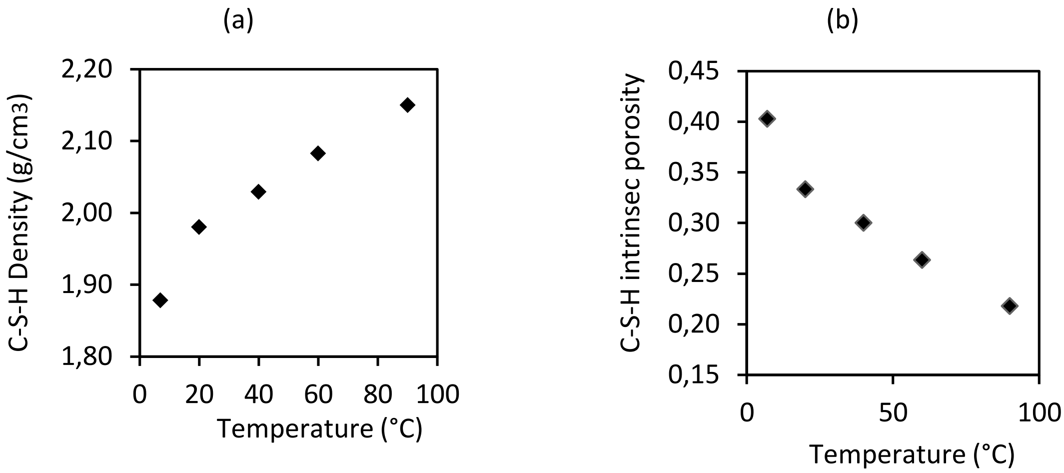

Figure 1: *(a) Variation of C-S-H density and (b) C-S-H intrinsic porosity with temperature*

Numerical modelling of desiccation cracking of clayey soil by using cohesive fracture method

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Keywords: Suction, evaporation, desiccation cracking, cohesive fracture, FEM

Abstract

This work presents a numerical study on the desiccation cracking process of clayey soil. The initiation and propagation of cracks were investigated by using a finite element code including damage-elastic cohesive fracture law to describe the behaviour of cracks. The coupling between the hydraulic behaviour (moisture transfers in the soil matrix and in the cracks) and the mechanical behaviour (volume change of the soil matrix and development of cracks) is also considered in the code. The results of laboratory experiment performed on clay soil, taken from the literature review, were used to evaluate the numerical modelling. The results show that the code is able to reproduce the main trends observed from the experiment (*i.e.* shrinkage related to drying, cracks development). Besides, the numerical simulation allows identifying the other phenomena, such as evolution of suction and stress related to drying or the development of a single crack.

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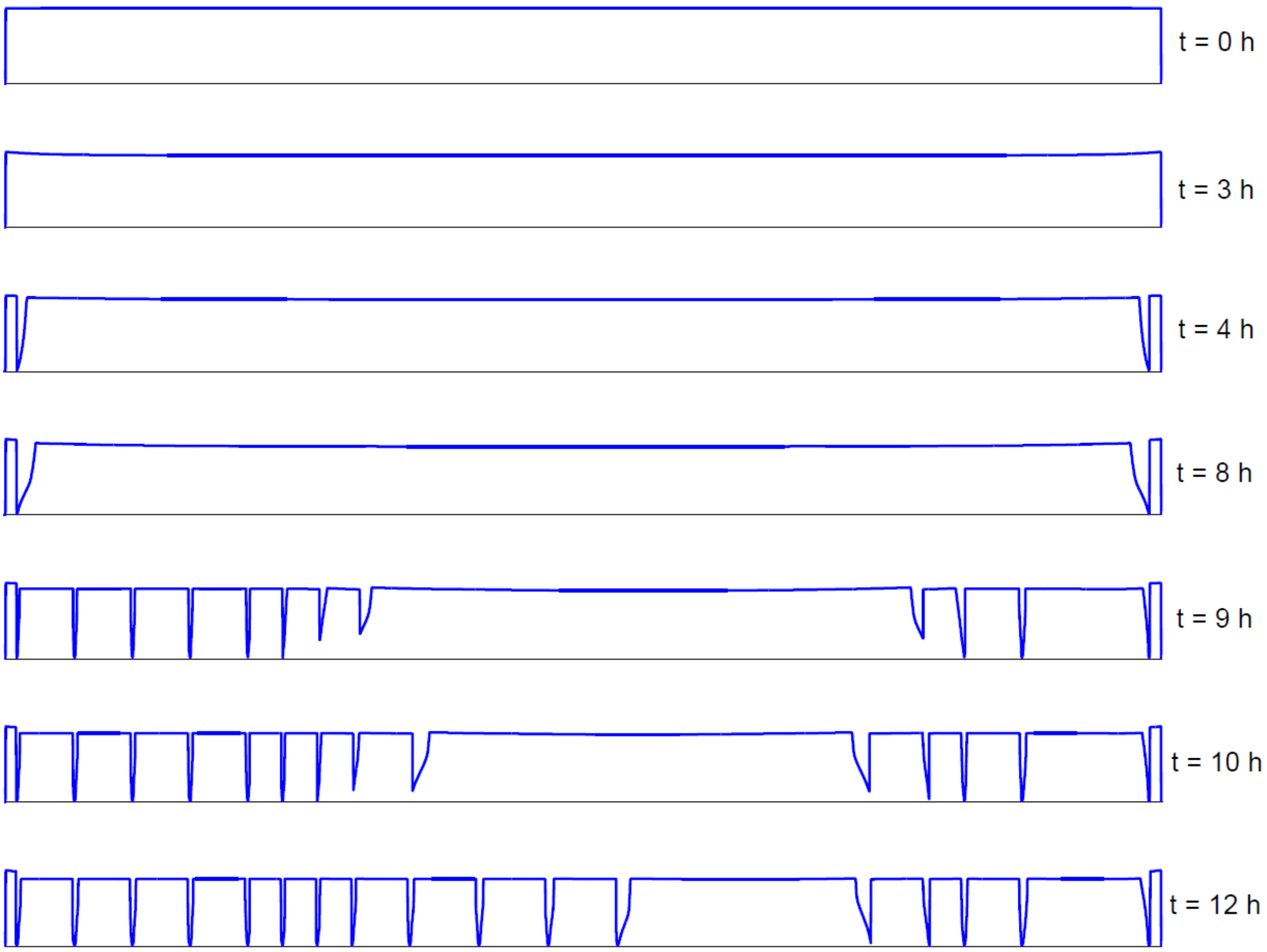

***Figure 1 :** Description of the cracks observed at various moments*

Damage models contributions on generation and development of failure zone around tunnels in quasi-brittle rocks

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Keywords: elastodamage model, softening, cohesive fractures, quasi-brittle rocks, damaged failure zone, instability, tunneling, numerical modeling

Abstract

The excavation of deep tunnels in quasi-brittle rocks creates a damaged area whose generation and development are important to determine the mechanical and hydraulic properties of the material around these structures. In general, with a continuum mechanics approach, the extension of this zone is estimated from a stress field calculated in elasticity or based on an elastic-plastic calculation ([1], [3]); while the first does not take into account the redistribution of stresses due to irreversible phenomena, the conventional elastoplasticity modelling seems insufficient to explain the geometry of the failure zone encountered in some cases of deep structures in quasi-brittle rocks. Observations suggest that the phenomena of softening damage are crucial to the development of these zones and must be considered for geotechnical simulations.

The simulations to be presented are performed with the numerical code *Porofis* ([4]), in plane strain ($\varepsilon_{zz} = 0$), with isotropic linear elasticity (E, ν) before the yielding occurrence, which is modelled according to the Drucker-Prager failure criterion, where the softening law varies depending on the elastoplasticity or elastodamage. Even if the parameters of both models can be calibrated to reproduce the same stress-strain curves under load in monotonous compression, these models can lead to different results, as shown in Figures 1a and 1b.

In the context of the feasibility study of the impact of a possible high-level and intermediate-level long lived waste disposal in the Callovo-Oxfordian claystone managed by Andra (the French National Radioactive Waste Management Agency) at the Underground Research Laboratory (URL) in Bure ([2]), a very weak anisotropy of the in-situ rock stress state has been introduced in the simulations, leading to the result reported in Figure 2.

On the other side, the propagation of fractures with the same weak anisotropy is analysed, inserting the cohesive fracture model ([5]) in a linear elastic matrix (E, ν). It is noticed a development of a brittle fractures system causing irreversible sliding (mode II cracking) among the mesh elements, with an expansion of totally or partially damaged joints as reported in Figure 3.

On one side, the presented research is intended to show the contribution of damage softening in the failure zone expansion around deep tunnels. On the other side, it is introduced a simulation of the fracture propagation while the tunnel internal pressure is progressively decreased. Further developments of the research will consist in a deeper study of the fracturing phenomena with the available models (e.g. parametrization, mesh size dependency) and eventually, establishing a coupling to simulate numerically a softening elastodamage model for the rock medium and a cohesive fracture model for the potential apertures

developing around the tunnel structure, in order to reproduce the conceptual model of damaged zone reported in Figure 4.

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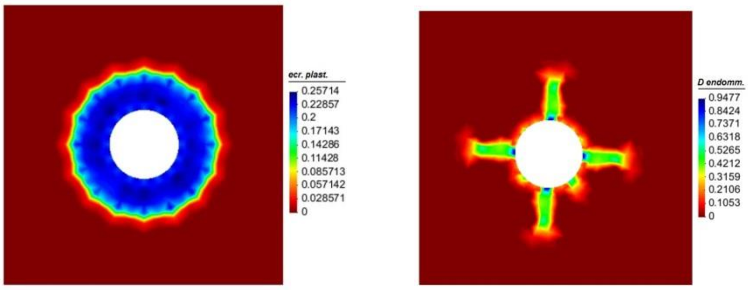

(a) ***(b)***

Figure 1: internal variable extension and values for the elastoplastic *(a)* and damage *(b)* softening models.

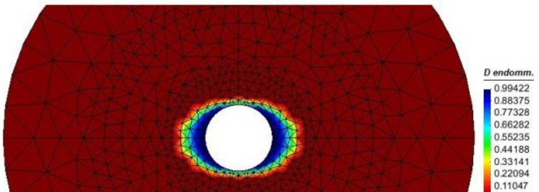

Figure 2: damage with weak stress anisotropy.

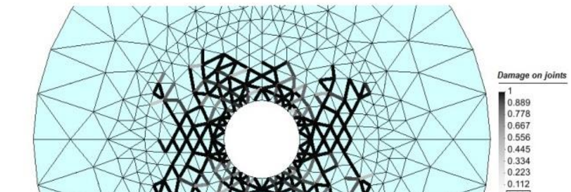

Figure 3: fractures network with weak stress anisotropy.

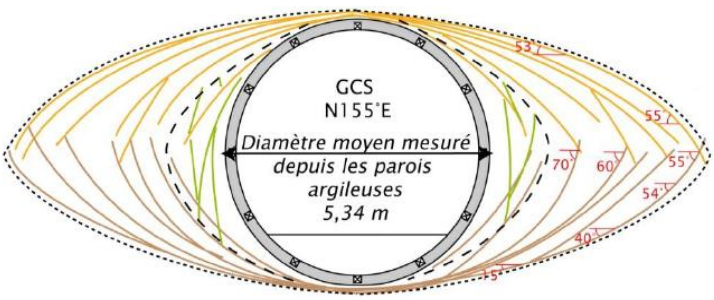

Figure 4: conceptual model of induced fractures and damaged zone at Andra URL for a tunnel excavated in a far-field stress state with weak anisotropy conditions. Modified after A .Noiret, Andra internal report, 2012.

Evolution of particles number due to breakage of a granular material

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Keywords: Particles number distribution, breakage, 1-D compression

Abstract

The basic constitutive properties of granular materials depend on their grading. Grain crushing modify the grain size distribution with a tendency for the percentage of fine material to increase.

This work shows the results of an experimental investigation consisting of a set of 1-D compression tests at different stress levels, on an artificial granular material, commonly known under the brand name LECA (Light Expanded Clay Aggregate). This material is characterized by a very low value of unit weight due to the grain intra-porosity (Figure 1) and therefore its particles break at lower levels of stress in comparison to *e.g.* natural sand (Casini *et al* 2013).

The main aims of this study are to understand how the breakage phenomenon evolves in terms of number of particles in each size range, *i.e.*, to identify which sizes are more susceptible to breakage, and any links existing between particle size evolution and the mechanical behaviour of the aggregate.

The number of particles in each size range is estimated dividing the total volume retained on a given sieve, by the nominal volume of the single particle, obtained assuming that the particle is a sphere. Figure 2 shows the evolution of the particle number in each size range with stress (de Bono & McDowell, 2016). In particular, the data reveal that, as crushing advances, the number of large particles decrease (Figure 2a) while the number of fine particles increases (Figure 2b). In Figure 3a three stress ranges are highlighted, dividing the compressibility curve divided in three characteristic parts; these are delimited by the yield stress and by the stress corresponding to the point of inflection (Figure 3a). Figure 3b shows the grain size distributions obtained at different applied maximum vertical stress, with the colours corresponding to the three stress ranges highlighted in Figure 3a. In phase 1, for stress lower than the yield stress, the number of particles in each size range does not change significantly because there is no significant breakage nor deformation. In phase 2, between the yield stress and the stress corresponding to the point of inflection, the number of large particles decreases while the number of small particles increases considerably. This phase is characterised by a large reduction of voids ratio. The large particles break and generate intermediate particles while medium sized particle bring into being small ones. small. In phase 3, at very high stress levels, breakage becomes more and more significant and the number of fine particles increases. This work is a part of a wider experimental work (*e.g.* Guida *et al.* 2016), still in progress, aimed at investigating in depth the multiscale effects of grain crushing: from the microscale of the single grain to the macroscale of the mechanical behaviour during 1-D compression. The three stress ranges introduced above correspond to characteristic behaviour

in the evolution of the aggregate's voids ratio (macroscale) but also in the number of particles in each size range (microscale) consistently to observations of the evolution of breakage proposed in the literature (*e.g.* Einav 2007).

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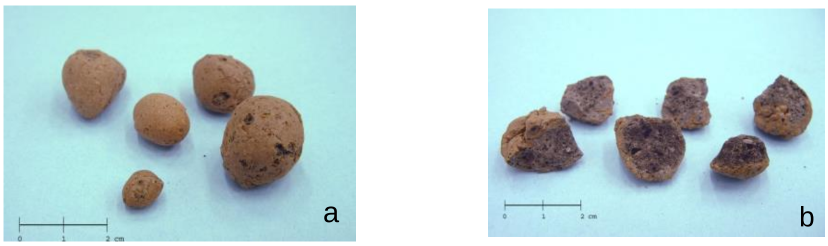

Figure 1: *LECA pellets: (a) whole, (b) broken with intra porosity.* (*Casini et al*, 2013)

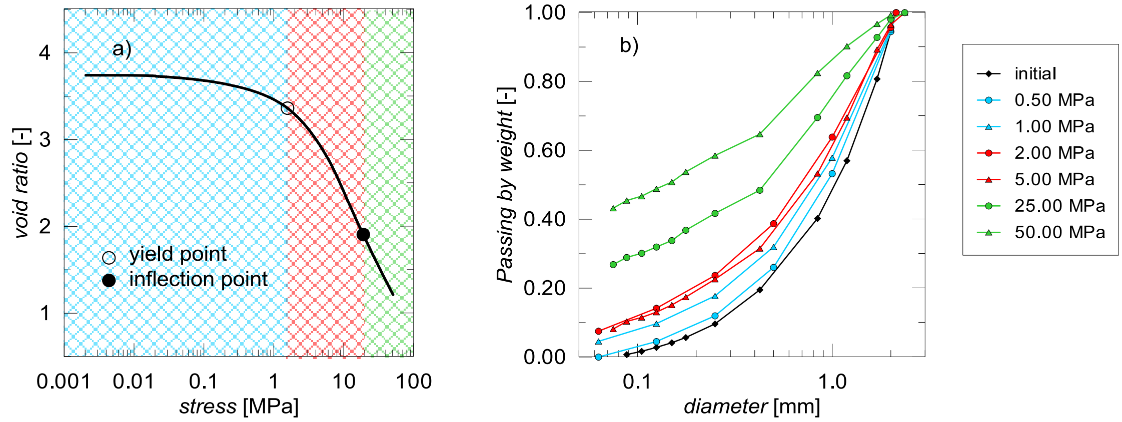

Figure 2: *Experimental results: (a)compressibility curve, (b)evolution of grain size distribution.*

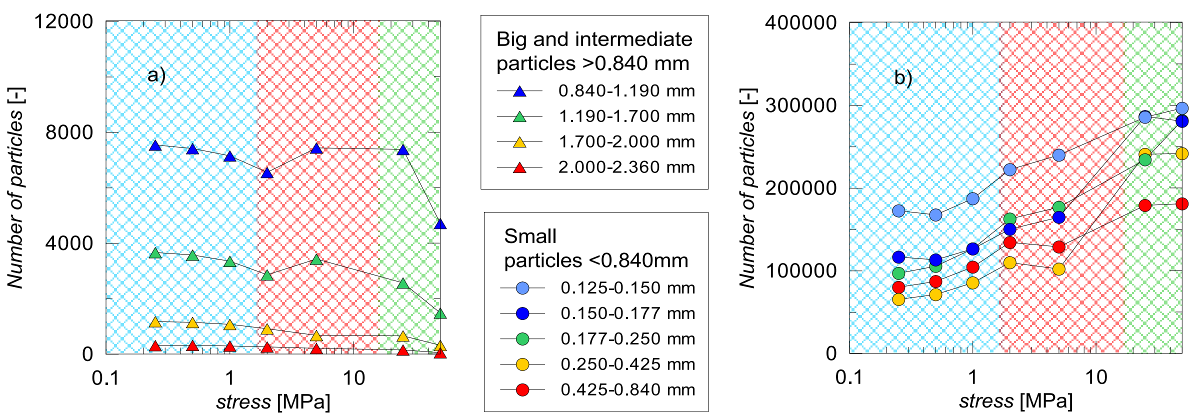

Figure 3: *Particles number distribution with stress level for (a)big and intermediate particles and (b) small particles.*

Grain and cement deformation in weakly cemented sands

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Keywords: sand; clay; quartz overgrowths; cementation; deformation bands; SEM; X-Ray CT

Abstract

The role of cementation type and degree on the generation and evolution of deformation bands in consolidated soils and rocks has not been yet fully understood. This work aims at a better understanding of the interaction between cementation and strain localisation. To do so, we focus on the micromechanics of cemented sand samples coming from natural outcrops and artificially made samples.

Our field case study is a Cretaceous deposit of weakly cemented sands, located in the southern France (Wibberley *et al.*, 2007). The sand outcrop offers a great exposure of deformation bands (Fig.1). The fieldwork is combined with laboratory production of artificially cemented sand samples that are used in comparison with the naturally cemented material collected from the field out of the deformation bands. In our artificial samples, we have chosen to test two different cement types: clay and calcite (Ismail *et al*., 2002). To better understand the role of cement in the deformation, we plan to perform a number of triaxial compression experiments on the artificially and naturally cemented samples.

In our work we are performing quali-quantitative measurements throughout Image Analysis, whose images are produced by two different techniques that work complementarily in the presented research: Scanning Electron Microscopy (SEM) and X-Ray Computed Tomography (XRCT). The first one provides 2D images at a resolution up to nm-scale enriched with information about the chemical composition of materials; the XRCT enables a 4D non-destructive inspection of materials at high resolution (μm) in condition of pre-, syn-, and post-*in situ* deformation.

First analyses of a sample coming from a deformation band in the outcrop and of material coming far from the band have shown local differences in the cement types within the weakly cemented outcrop: while a mixture of clays connects the grains with menisci bonds in the naturally cemented samples far from the deformation bands (Fig. 2), a singular 50 cm thick deformation band crossing partially the deposit reveals the presence of quartz overgrowths (Fig.3) together with the clay mixture. The quartz layers result in some parts “disturbed” by the presence of clay and of other inclusions. Moreover, the rounded to well-rounded grains outside the deformation bands (Fig. 4) are replaced by broken angular grains and tiny quartz fragments inside the band (Fig. 5), which can be considered to be regarded as traces of deformation. Trying to explain the origin of the quartz overgrowths cementation, which is weakly supported by the geothermic condition of the field area during deposition, we are now wondering whether the thinner deformation bands, broadly distributed in the deposit, share similar characteristics with the thick one analysed.

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Figures

Fig. 1

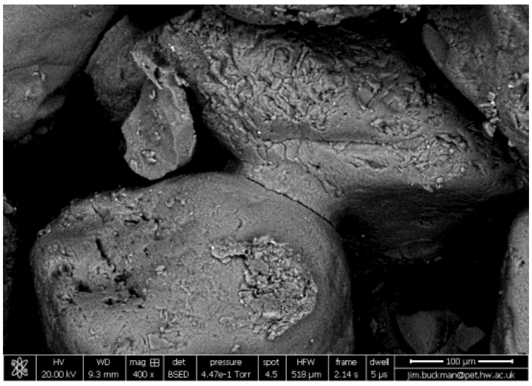

Fig. 2

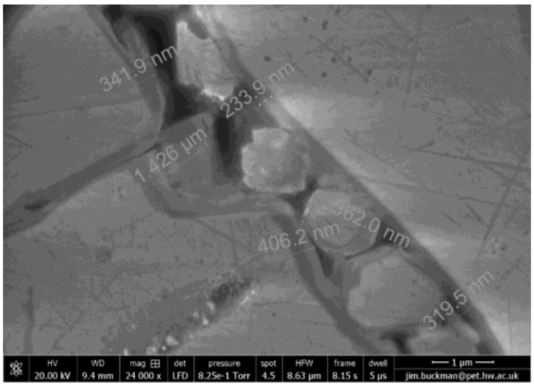

Fig. 3

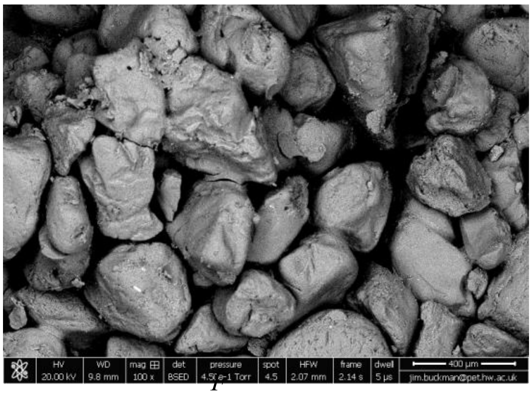

Fig. 4

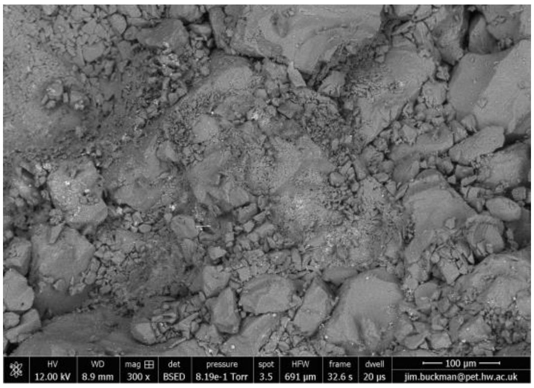

Fig. 5

Dependence of suction and its recent history on small strain stiffness of unsaturated silty clay

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Keywords: unsaturated soils, small strain stiffness, suction

Abstract

The main objective of the proposed research is to study the effects of recent stress and suction history on the initial stiffness and on the stiffness decay curve of unsaturated soil. Ng and Xu (2012) studied the behaviour of coarse-grained soils, while the current research deals with a silty clay. Results from this laboratory study are to be used for calibration of the hypoplastic model by Wong and Mašín (2014).

Two reconstituted triaxial samples (a loess), 70 mm and 38 mm in diameter, were tested. The 70 mm sample was tested in a double wall cell triaxial system, while the 38 mm was tested in a standard triaxial cell. Both samples were fitted with axial LVDTs. For measuring the volume of the sample, the 38 mm sample was fitted also with radial LVDT. The G_0 was measured by bender elements mounted in the pedestals in the case of 70 mm diameter sample and on the side of the sample in the case of 38 mm diameter sample (vertically polarized, G_{vh}=G_{hv}). To apply the suction, the axis translation technique is used. For controlling pore-water pressure, pore-air pressure and cell pressure the pressure/volume controllers are used. The applied stress paths are shown in Fig. 1. 70 mm and 38 mm sample is in red and in blue, respectively. A small drained shear probe is taken (ranging from 30 to 50 kPa), followed by unloading, at each step of the stress/suction condition change. See black arrows in Fig.1. The Fig. 2 shows an example of influence of suction and its history on G_0 and the shear modulus reduction curve for 70 mm diameter sample. The data show an increase of stiffness related to increase of suction and its history. The plateau in the data from LVDT measurement (square shaped points), which doesn't correspond to the bender element measurement, is most probably caused by tilting or bending of the sample as a result of the loadcell-specimen connection (e.g. Gasparre et al., 2014).

Acknowledgments

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Figures

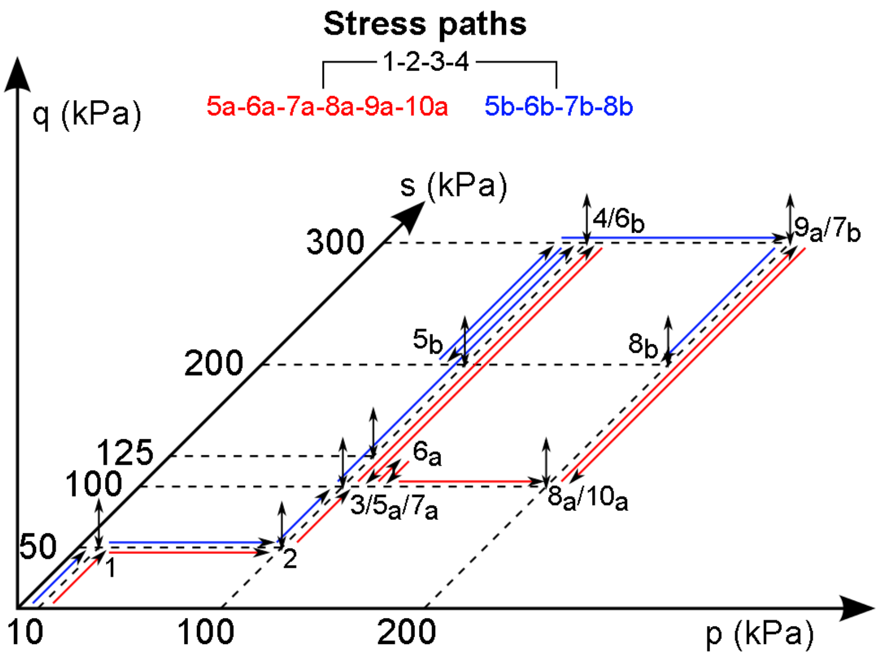

Figure 1: Applied stress paths; red - 70mm diameter, blue - 38mm diameter.

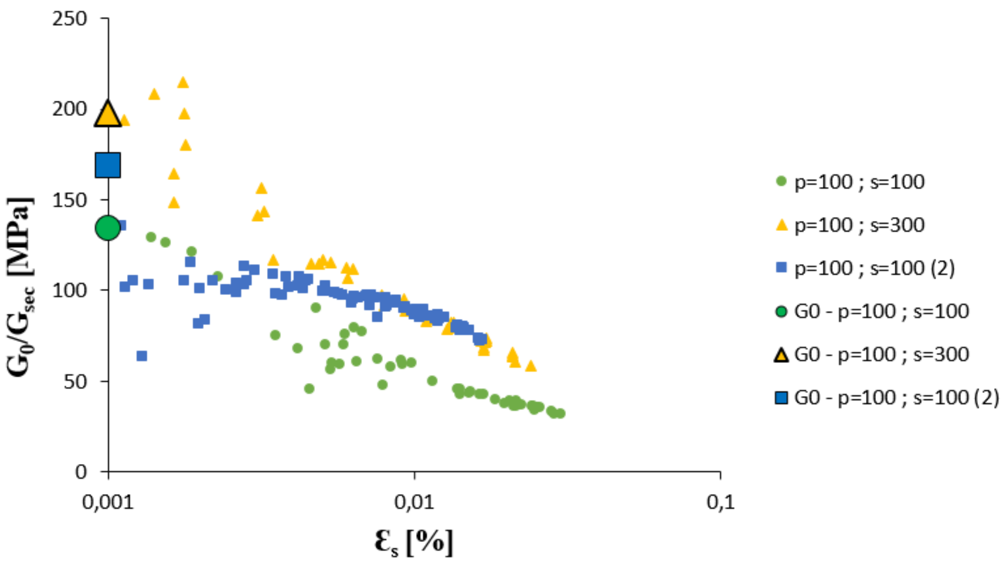

Figure 2: Effects of suction and its history on G_0 and shear modulus reduction curve ; stress path = 3-4-5_a (see Fig. 1).

A water retention model for compacted bentonites

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Keywords: Unsaturated soil mechanics, water retention behaviour, expansive soils, microstructure

Abstract

Bentonite-based materials are studied as potential barriers for the geological disposal of radioactive waste. Under repository conditions, the engineered barrier experiences hydration from the saturated host rock. Because of the existence of technological gaps, the periphery of the engineered barrier swells under free conditions first. Once that contact between bentonite and the host rock is reached, hydration continues with important redistribution in bentonite dry density. Experimental data from the literature show that the water retention properties of the bentonite barrier significantly evolve along such stress paths. Based on observations of the material double structure and the water retention mechanisms in compacted bentonites, a new water retention model is proposed. The model considers adsorbed water in the microstructure and capillary water in the inter-aggregate porosity. The model is calibrated and validated against experimental data taken from the literature, showing good capabilities in capturing the main features of the water retention behaviour of compacted bentonites, including the evolution of the water retention properties upon free swelling (Figure 1). The model provides a better understanding of competing effects of volume change and water uptake observed during hydration under free swelling conditions.

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Figures

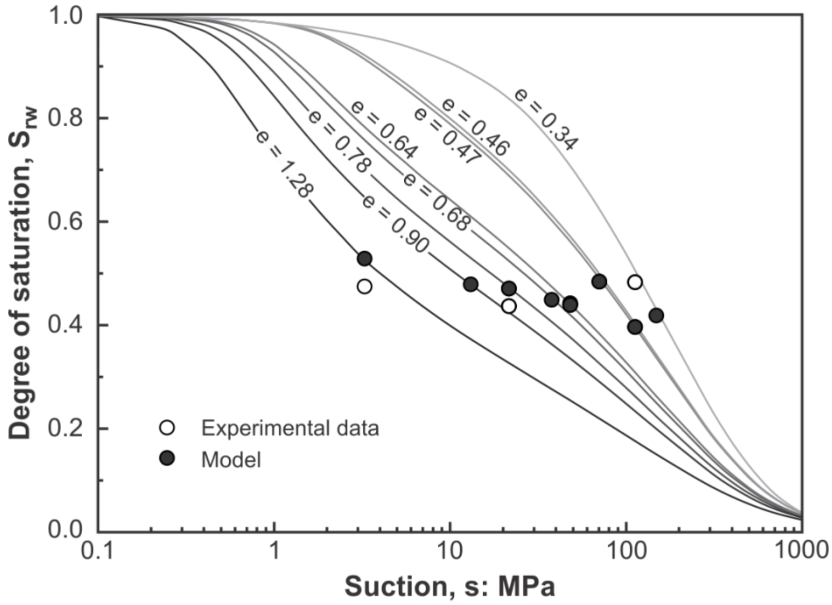

Figure 1: *Comparison between experimental data (Gatabin et al. 2016) and model predictions. Wetting path under unconfined conditions.*

Hypoplastic model for clays with anisotropic state boundary surface

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Keywords: hypoplasticity, constitutive modelling, soft clay, anisotropy

Abstract

The stress-strain behaviour of soft natural clays is complex, and one of their features is that they develop significant degree of anisotropy of the fabric during deposition and one-dimensional consolidation. The objective of the present research is to incorporate strength anisotropy into the latest version of a hypoplastic model for clays (Mašín, 2014), thus expanding the capabilities of the model.

Anisotropic state boundary surface has been implemented into the model, which was possible thanks to the fact that the hypoplastic model allows for explicit formulation of the state boundary surface. The model was used to simulate laboratory experiments on soft marine clays involved in Nicoll highway collapse in Singapore by Corral (2010). It has been shown that by skewing the ASBS the model predicts correctly the ultimate strength of the material. However, skewing of the SBS proved not to be enough to predict fabric-dependent stiffness evolution with strain. In the coming work, it will be necessary to enhance predictions of stiffness decrease in extension to obtain results which agree better with laboratory experiments.

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Acknowledgement

The research is supported by a grant of the Charles University Grant Agency: 1075516.

Figures

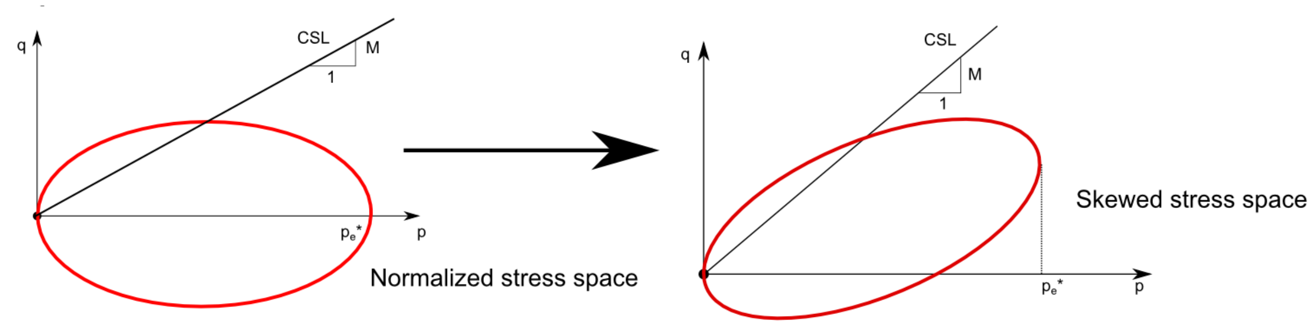

***Figure 1**: Proposed approach for skewing of the stress space, thus skewing the ASBS.*

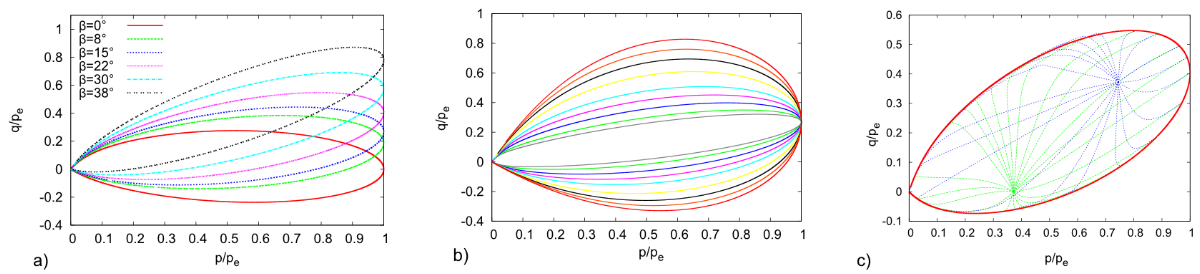

***Figure 2:** Results of the model: a) SBS of the newly developed model with various values of rotation, b) SBS rotated by β=22° with various values of critical state friction angle (ranging from φ=14° to φ=39°). c) Normalized stress paths starting from two arbitrary states leading to an asymptotic state, thus forming asymptotic state boundary surface.*

Determination of the swelling potential of the clayey soils in engineering practice

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Keywords: swelling potential, free swelling, cation exchange capacity CEC, degree of saturation

Abstract

The free swell strains are one of the most representative properties in the estimation of swelling behaviour of the soil. The oedometer was used to measure the free swelling and thus the swelling potential of the clayey saturated soils (except of V4 – Sr 0,9 and V9 – Sr 0,8). The results were compared with the unsaturated silty clay (V1 natural texture V2 reconstituted), where no swelling was expected. The structure of the clay minerals e.g. montmorillonite influences the swelling behaviour as well. The strains were correlated to mineralogical properties (cation exchange capacity CEC - as an indicator of the expansive minerals in the soil, and X-Ray diffraction), to suction (using the filter paper method - ASTM D 5298-03) and to degree of saturation (Sr). Generally, the swelling potential is supposed to increase/decrease as CEC, content of montmorillonite or suction increases/decreases. However, the values of free swell strains were not consistent with the mineralogical properties (CEC) and degree of saturation (Fig. 1). The obtained values, the swelling potential and the origin of the deformation of the tested soil samples will be dealt with in the poster.

Acknowledgement

The research was supported by the TAČR: TA04021261 and by the GAUK 1050216.

Figures

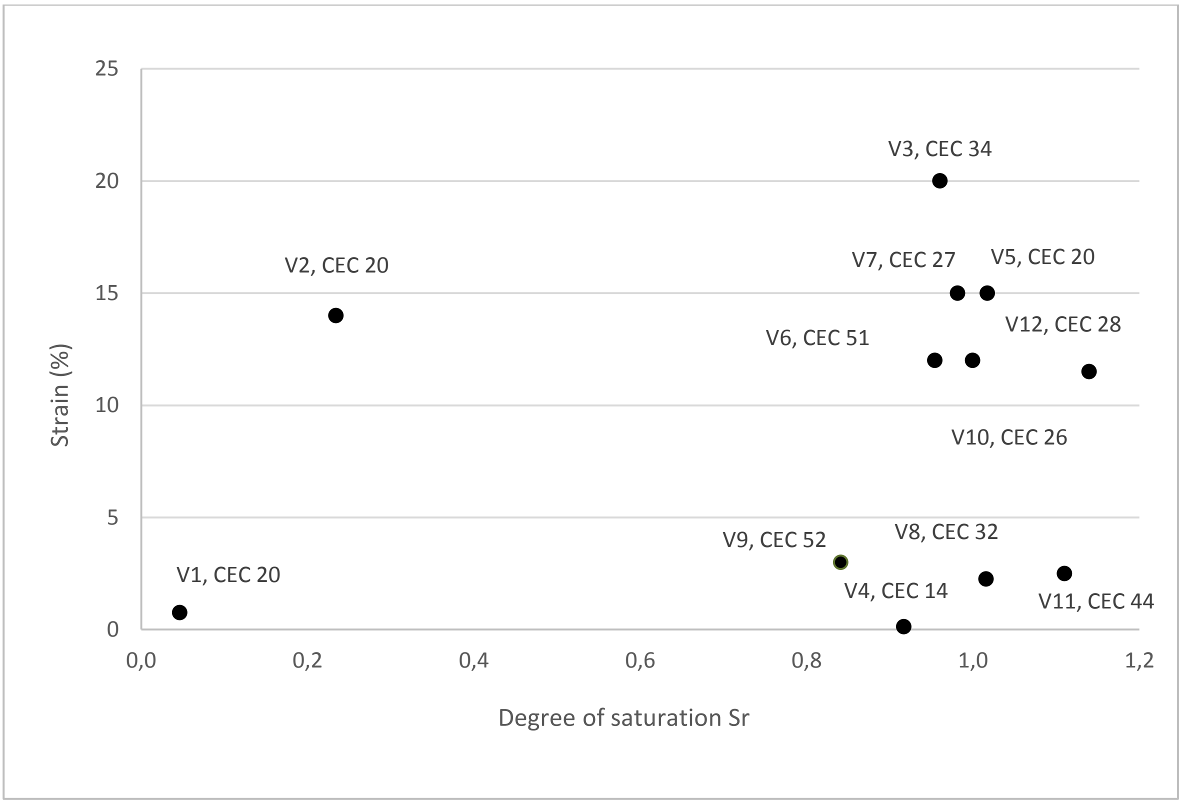

Figure 1: *The values of strain, degree of saturation and cation exchange capacity CEC.*

Influence of CO_2-induced geochemical reactions on the oolitic limestone: a lab-scale investigation

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Keywords: oolitic limestone; supercritical CO_2; brine; ESEM

Abstract

This pilot study aims at gaining insights into how the physical and petrophysical properties of brine-saturated carbonate rock systems change due to CO_2 injection, with implications for places where carbonate rocks – depending on their porosity and permeability - form either the cap rock or the host rock of the storage site. In particular, we are interested in the influence of CO_2 -induced geochemical reactions on the mechanical integrity of an oolitic limestone being subjected to typical reservoir conditions at the laboratory scale. To achieve this target, we perform CO_2 high pressure - high temperature tests on brine saturated samples, to identify changes in the fluid chemistry and the limestone mineralogy upon the completion of each test. By preparing pre- and post-treatment thin sections from regions close to the sample edges we aim at identifying possible deformation micro-processes and mineral changes that could occur due to the thermo-chemo-mechanical loading of the samples.

SEM imaging on the oolitic limestone before the high pressure-high temperature tests indicated that this is a low porosity material. Calcite cement grew into the pore space from the ooids' margin, as a fine-grained radially orientated cement phase, followed by a coarser pore occluding cement. However, calcite was not everywhere well-attached to the ooids. Moreover, micro-porosity and pressure solution were identified within some of the ooids and at their edges, respectively.

On the one hand, grain-scale investigations based on thin section observations (SEM imaging) on a brine-saturated limestone sample exposed to 230 bar CO_2 pressure and to 37.5^{o} C (i.e. supercritical conditions) for a total time of 2 weeks, revealed no obvious fractures linked with the thermo-chemo-mechanical loading of the sample. Micro-porosity in a few ooids together with occasional big voids in cement between ooids were identified locally in the post-deformation/treatment sample; however, similar observations were also made in the pre-treatment sample. Moreover, a few sporadic fractures along ooids were identified in both pre- and post-deformation samples. All micro-scale observations were made in regions 1-3 mm from the sample edges, indicating no actual grain-scale deformation. On the other hand, the increase in concentration of calcium ions in the post-treatment brine was linked to dissolution

of the limestone, which possibly took place along the surface of the sample. Thus, we wish to argue that under the current test conditions (230 bar, 37.5^{o} C, 2 weeks exposure) CO_2 does not much damage this repository. We are currently performing further research on different conditions (particularly long exposure and higher brine -rock rations that can be linked with faster dissolution of calcite) in order to understand the dominant CO_2 sequestration mechanism in oolitic limestone-containing reservoirs as well as the effects of CO_2 injection on their mechanical integrity.

This pilot project has been funded by the Heriot-Watt Energy Academy 2015 Fledge Award.

DEM investigation of stress and strain evolution around displacement piles in sand

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Keywords: DEM, Grain Crushing, Pile penetration, Boundary Value Problem

Abstract

A three-dimensional discrete element model is used to investigate the effect of grain crushing on the tip resistance measured by instrumented piles in a calibration chamber. The particles of the discrete model have a size-dependent crushing resistance whose material parameters were calibrated against an oedometer test and single grain crushing experiments, with additional validation by element tests. The numerical pile penetration tests agree encouragingly well with the instrumented pile experiments.

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Figures

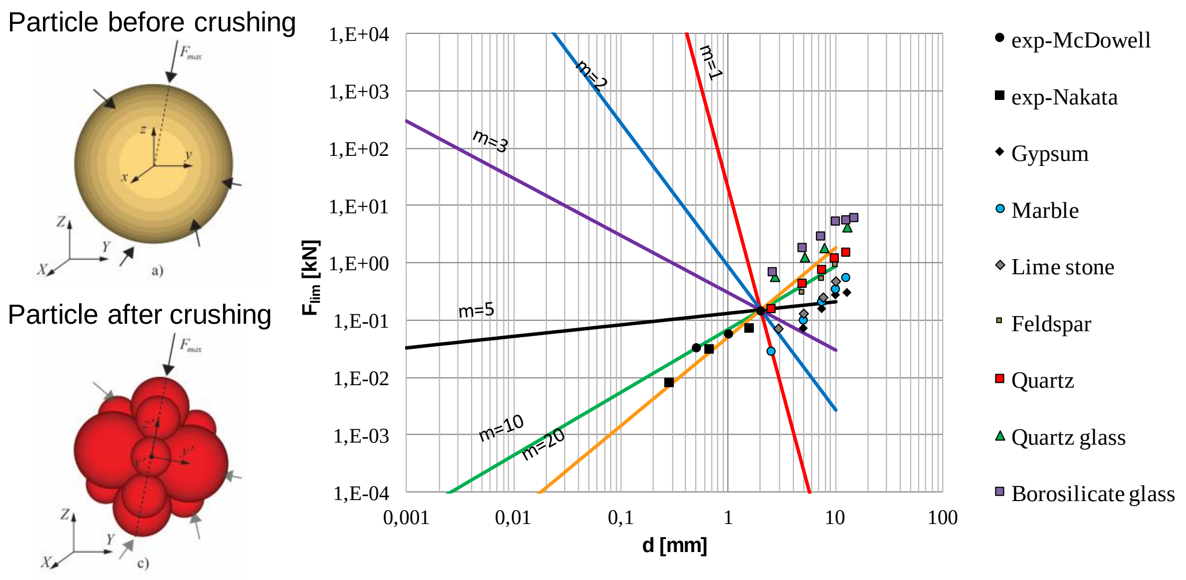

Figure 1: *Particle limit contact force as a function of particle diameter, where* $F_{lim} = _{(lim,0)}(d/Nd_0)^{\wedge}(-3/m)A$*. Also shown are single grain crushing experiments by Yashima et al. (1987), Nakata et al. (2001) and McDowell (2002) after Ciantia et al. (2015).*

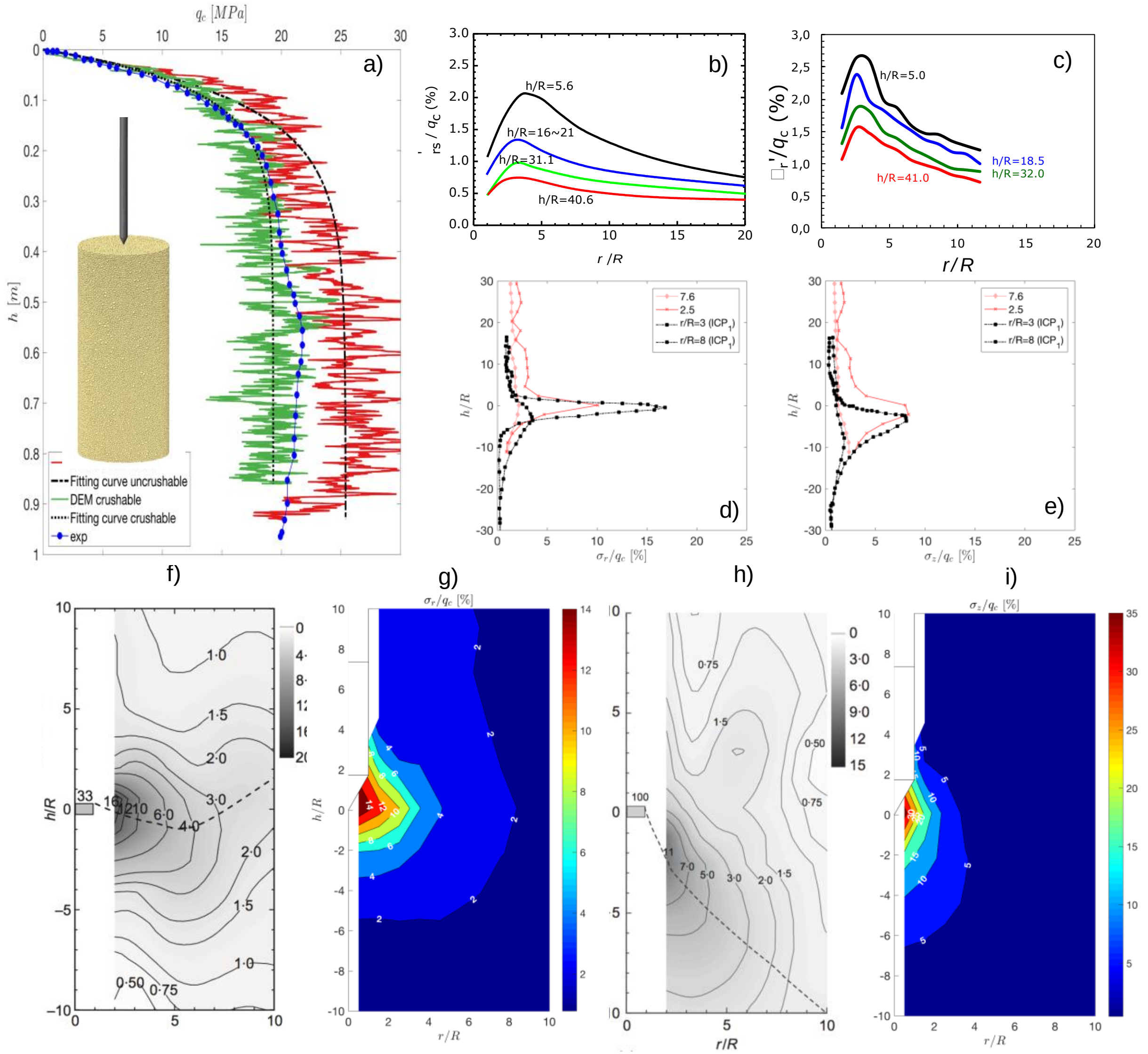

Figure 2: *a) DEM pile tip resistance predictions for crushable and uncrushable dense assemblies compared to CC experiments on NE34 sand. Both raw DEM and smoothed 'fitted' curves are shown; Top: profiles of* σ'_r/q_c *with radius (r) for 4 levels (h) above the tip; b) experiments, c) DEM predictions. Note* q_c*=CPT resistance, R= pile radius. Mid: profiles d) & e) show* σ'_r/q_c *&* σ'_z/q_c *against h/R, experiments & DEM model for paired r/R locations. Bottom: Experimental & DEM contour plots for* σ'_r/q_c *(f & g) and* σ'_z/q_c *(h & i) in r/R, h/R space.*

Critical and residual shear strength of soils from Dobkovičky landslide in Central Bohemian uplands

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Keywords: critical shear strength, residual shear strength

Abstract

The objective of this research is to evaluate the critical and residual shear strength of soils from Dobkovičky landslide, to be used later for numerical modelling of the slope stability using probabilistic methods. After heavy rains the landslide was activated on June 6th 2013, damaging D8 motorway under construction (Fig. 1). The laboratory tests were carried out on two types of soils, clay and tuff, both obtained from the slip surface. The samples were obtained during the site investigation in 2015. Critical and residual friction angles were evaluated on both samples. Triaxial CIUP tests and shearbox tests were used for evaluating critical parameters and ring shear apparatus was used for residual parameters.

In this poster, preparation of specimens, test procedures and experimental results are presented for each type of laboratory test.

Figures

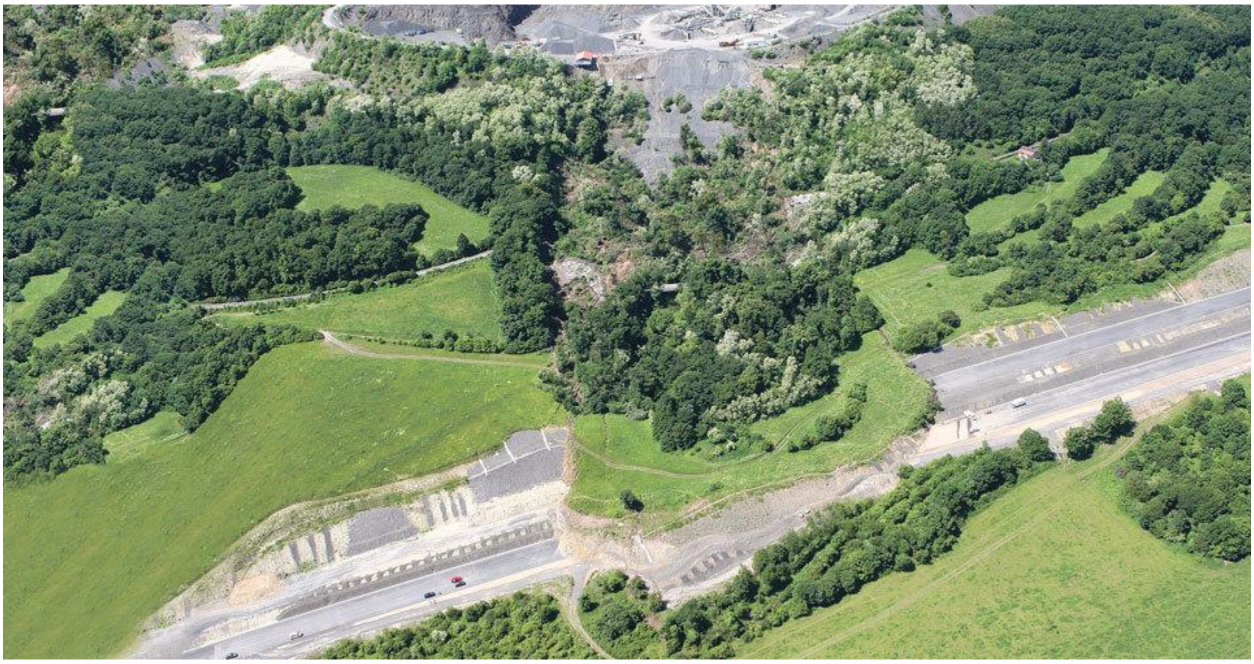

Figure 1 : *Dobkovičky landslide, photo 2013*

Hydration kinetics of a class G oil well cement paste under various temperature and pressure conditions

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Keywords: Oil well cement, hydration kinetics.

Introduction

Cement sheath plays a major role in oil wells, assuring zonal isolation, well stability and protecting the steel casing from corrosion (Fig. 1 [1]). The physical and mechanical properties of this cement-based structure largely depend upon the hydration degree. As shown in Fig. 2, the hydration reactions are highly dependent on the curing conditions, namely pressure and temperature, with values that can span over a wide range.

We describe the kinetics of phase transformation, from the main clinker components to the final hydration product, based on a general-purpose solid-state kinetics equation. The proposed expression yields accurate fits that closely match the observed experimental hydration degree as determined from isothermal calorimetry.

Experimental procedure

The hydration degree is determined by means of isothermal calorimetry, where the evolved heat is measured and converted to hydration degree by comparison to the total heat evolved for complete hydration:

$$\alpha(t) = \frac{\sum Q_i(t)}{\sum Q_i(t \to \infty)}$$

where the summation is over the clinker components. A wide set of data has been analyzed for the determination of the hydration kinetics parameters. When possible, results from the literature have been integrated [2,3]. The set includes temperatures ranging from 7 to 60°C and pressures ranging from 0.1 to 45 MPa. All data corresponds to API class G cement pastes with a water-cement ratio of 0.44. The slight differences in composition have been accounted for in the determination of the hydration degrees.

Modelling

The kinetics will be described by the following equation [4]:

$$\frac{d\alpha}{dt} = k'.\alpha^m.(1-\alpha)^n.(-\ln(1-\alpha))^p$$

where the parameters k', m, n, p are to be determined. This equation can reproduce a wide variety of phase transformation kinetics by assigning adequate values to the aforementioned parameters. The rate-controlling mechanisms can be best understood by analyzing the relative importance of different terms in limiting cases of small or large α.

From the regression fit of the experimental results, we can derive a set of parameters that reproduces the observed data with an overall mean error of 4%. A sample fit is presented in Fig. 3 for relevant values of pressure and temperature. As expected, the reactions are activated by both the temperature and pressure. The effect of temperature is predominant in the range of values considered.

Conclusion

A new kinetics equation has been proposed, that can accurately reproduce experimental observations without the need for explicit differentiation of rate controlling mechanisms. Furthermore, it can be shown that the transition of mechanism control is smooth.

Additional parameters are to be added in the formulation, to account for cement composition, fineness and water/cement ratio. Individual hydration curves for different components are to be determined from the analysis of rich data sets of hydration curves.

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Figures

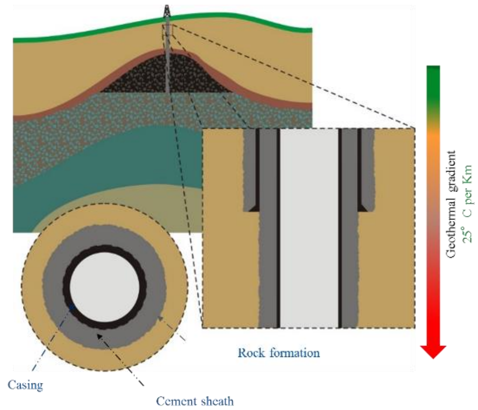

Figure 1 : *Oil well schematic representation.*

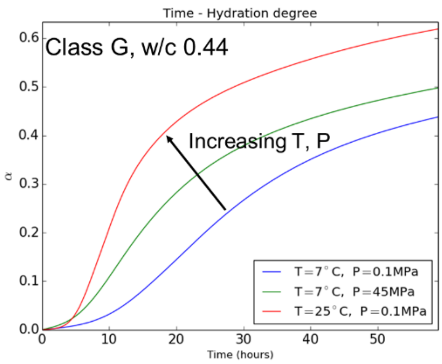

Figure 2 : *Effect of pressure and temperature.*

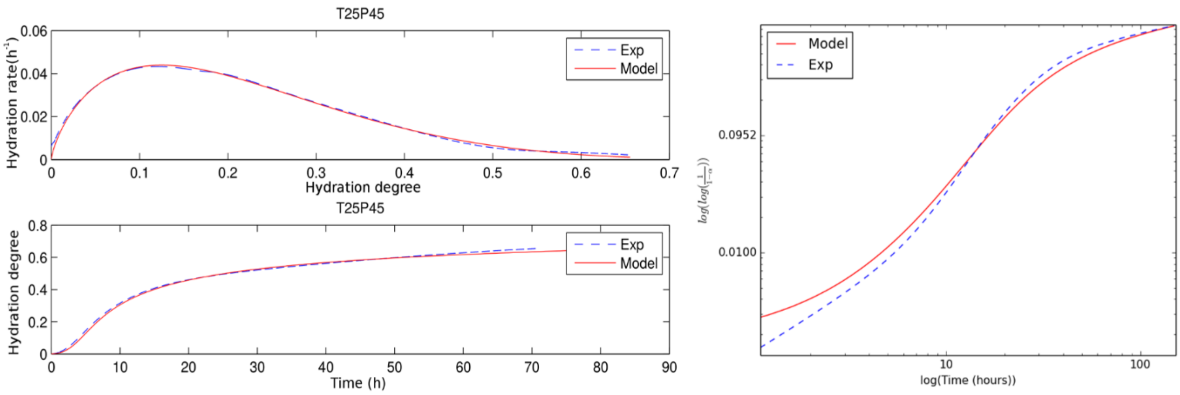

Figure 3 : *Validation fit with an independent test.*

Pore pressure diffusion in some basic rock mechanics experiments

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Keywords: analytical solution, thermo-hydro-mechanic experiments, claystone, radioactive waste, poroelasticity

Abstract

When determining the poro-thermo-elastic properties of porous materials, elementary experiments are performed on samples under various mechanical, hydraulic and thermal loadings. A necessary condition hereby is the homogeneity of the pore pressure field in the sample throughout the experiment. However in reality, the pore-pressures generated in the centre of the specimen needs a certain time to diffuse and equilibrate with the imposed pressures at the boundaries. This results in a non-homogeneous pore pressure distribution along the sample and induces an error in the evaluation of the material parameters. This problem is particularly important in testing low permeability geomaterials with a permeability in the order of 10^{-19} m² or smaller, such as the Callovo Oxfordian claystone studied in the context of radioactive waste storage [1, 2, 3].

In this work, pore pressure dissipation in isotropic thermo-poro-elastic materials is analysed through analytical and numerical calculations, for samples submitted to isotropic stress or temperature changes with one dimensional drainage. Different THM loading paths corresponding to basic poromechanics laboratory tests are applied.

An analytical solution describing the changes in pore pressure with respect to time and location is presented for a sample under combined loading paths of different rates and directions. This solution permits to evaluate the error in the measurement of material parameters in various poromechanical experiments. Particular solutions are presented for widely used experiments: isotropic drained compression test, unjacketed compression test, pore pressure loading test under constant confining stress and drained heating test. An example of the generated pore pressure and the resulting volumetric strain during drained isotropic compression tests with two different loading paths is presented in Figure 1. We can observe that under constant rate loading (Figure 1a) the excess pore pressures tends to reach a given constant pressure after some time, once generated and dissipated pressures are equilibrated (Figure 1b, blue path). The measured volumetric strains at the sample centre provide hence a tangent modulus that changes over time and that is equivalent to the input material parameter K_{param} only once pore pressures remain constant (Figure 1c, blue path).

Undrained tests are simulated with a one dimensional finite difference model taking into account the “dead” volume of the drainage system of the triaxial cell connected to the sample. The pore pressure boundary condition corresponding to this dead volume is hereby modelled

with the fluid mass conservation equation and takes into account the error resulting from the reservoir and fluid deformability [4]. This simulation provides an estimation of the optimal conditions for measuring the undrained thermo-poro-elastic parameters of porous materials.

Finally, a parameter study is presented to show the influence of both the material parameters of the Callovo Oxfordian claystone and of the testing device geometry on the time and rate effects previously discussed. Depending on these factors, the generated pore pressures, the relevant loading durations and the measurement errors that should be considered in an experimental program can be easily evaluated.

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Figures

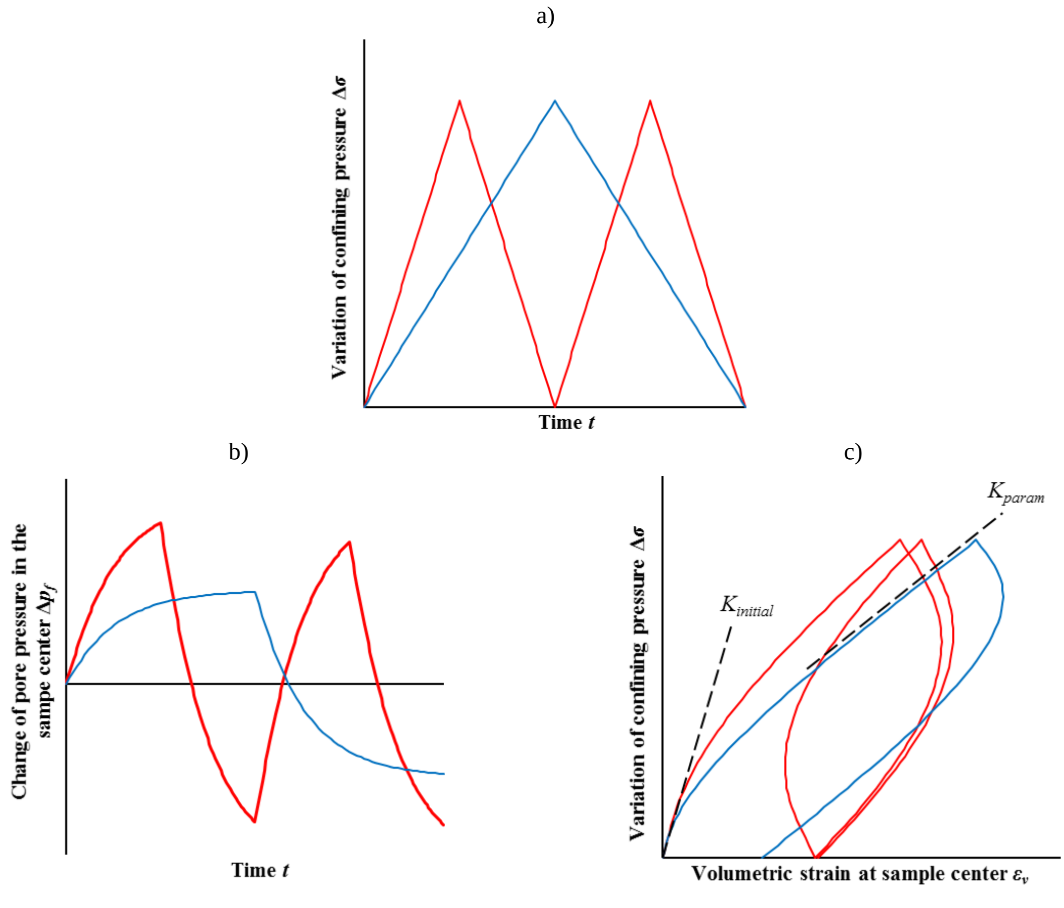

Figure 1: *Examplary simulation of drained test under two different loading rates (a), generated pore pressures (b) and resulting deformations (c).*

A pore-scale approach for hydromechanical couplings of partially saturated graunlar materials

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Keywords: Granular material, hydromechanical coupling, discrete element method, two-phase flow, pore-scale network

Abstract

The situation of two immiscible fluids going through a deformable granular material is widely encountered in nature and in many areas of engineering and science. To understand the physical evolution of the multiphase system is of great importance for the applications. In this contribution, we propose a pore-scale numerical model to simulate the hydro-mechanical couplings. The underlying idea is to combine a pore-scale network and the discrete element method (DEM) for the fluid phases and the solid phase, respectively.

In this study, the method is applied to the quasi-static regime in dense random polydisperse sphere packings created with DEM [1], aiming at simulating the primary drainage of a nonwetting-wetting-solid (NW-W-S) phases system. The pore space of fluids (NW/W phases) is decomposed into pore bodies connected with narrow throats using the Regular Triangular method [2], by which an explicit link network between the geometry of pore space and the position of solid grains is established. The criterion for invading a local pore is formulated based on Mayer-Stowe-Princen (MS-P) method [3, 4], which employs the balances of forces on the fluids interface near the throat [5]. Drainage occurs by a recursive invasion of the pores when the capillary pressure exceeds the local threshold value (entry capillary pressure). Under the pendular regime, the W-phase menisci between grains are also considered, in which the liquid bridge model [6, 7] is employed and combined with the network. The capillary forces induced by the fluids pressure and interfacial tension are derived and taken into account when solving the motion of the solid grains with the DEM. The macro-scale deformation of solid skeleton finally is obtained.

We apply the model to access the size effects and boundary effects on primary drainage when testing small samples (see Fig.1) [8]. Repeated simulations shows that the standard deviation of the saturation follows a simple variance reduction law with increasing sample size. Standard deviation should not be the unique criterion for evaluating the representativity. The sample size can be the cause of significant bias in the average result. We find that at least 20,000 spheres must be used in order to reduce the bias below 0.02 in terms of the saturation for a give capillary pressure. For the boundary effects, we found that the preferential invasion occurring along the boundaries led to more robust evaluation of the capillary pressure - saturation relations, else the phase distribution always showed a strong gradient of saturation.

We examine Bishop's effective stress parameter χ. The evolution of χ is obtained from macroscopic deformation and microscopic variables, where the macro-scopic expression uses the definition of effective stress and the microscopic expression is based on the contact stress between solid grains. The results show that both ways lead to similar results (the error is less

than 10%), as shown in Fig.2 [9]. We conclude that the micro-mechanical stress can be used to estimate the effective stress of the unsaturated granular materials.

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Figures

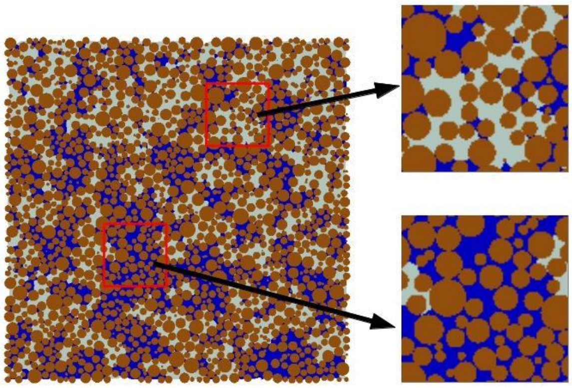

Figure 1 : *A slice through a sample at 0.4 of saturation (the NW phase invades from the top and W phase recedes from the bottom), in which strong capillary fingering can be observed*

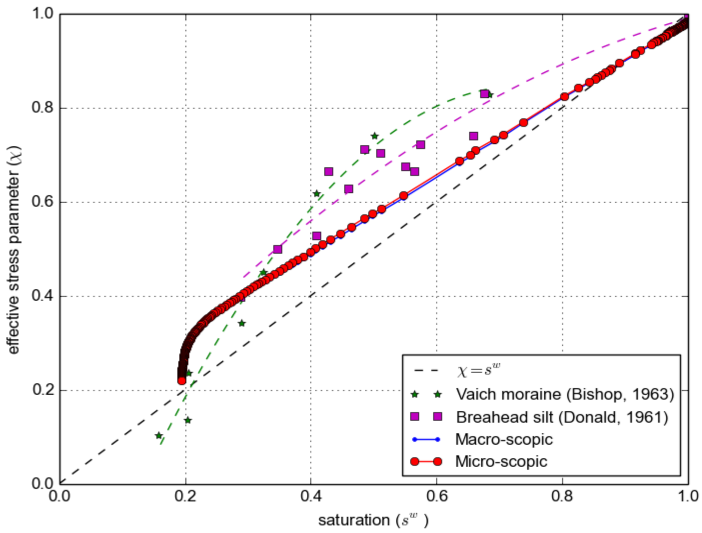

Figure 2 : *Variation of effective stress parameter χ with saturation for simulation results and experimental data. Simulation values are calculated from drainage test of a dense packing (40,000 spheres) under the oedometer test conditions.*

B free finite element approach for saturated porous media

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Keywords: Finite Element Method, B free, saturated porous media, consolidation

Abstract

The range of interesting problems involving porous media has increased dramatically in recent years. These problems might arise from different environmental fields like agriculture, petroleum engineering or natural hazards, to mention a few [1-2]. A key aspect in order to develop accurate models, capable to reproduce the principal features of this wide class of phenomena is the adequate description of multiphase porous media. Such multiphase materials can be properly described within the thermodynamically consistent theory of porous media (TPM), where all constituents are assumed to occupy simultaneously the space [3].

In order to obtain accurate, robust and efficient solutions of the coupled partial differential equations that come up from TPM, numerical techniques are usually required. In this context the finite element method is one that has achieved significant results [4, 5].

Due to the widespread application of the finite element technique in engineering modeling, it is of great relevance how this numerical procedure is taught in graduate and undergraduate courses. In this context the B free finite element approach recently proposed in [6] is of paramount significance. The main ideas behind the B free finite element approach are the following ones:

1. Use of Voigt algebra is avoided within B free approach. Under Voigt algebra second order symmetric tensors in 3 dimensions are represented as a 6 dimensional vectors and a fourth-order symmetric tensor is rewritten as a 6x6 matrix. Instead of this vectorization approach, which might be error prone [6], the so called B free approach is tensor based. Only vectors and second order tensors and their natural operations are considered, at least in solid mechanics. Fourth order tensors are employed through development of the finite element equations, however the Cartesian components of such type of tensors will never appear within the implementation.

2. From the previous point it can be inferred that the strain operator B, which relates the strain vector (increment) with the nodal displacements (increment), is not required. In the same way, the constitutive D matrix, appearing in the tangent stiffness matrix in the standard finite element implementation is also not required.

In this work [7] the B free finite element approach is applied to the governing equations describing the consolidation process in saturated poroelastic medium with intrinsically incompressible solid and fluid phases. Under this approach, where Voigt notation is avoided,

the finite element equilibrium equations and the linearization of the coupled governing equations are fully derived using tensor algebra. In order to assess the B free approach for the consolidation equations, direct comparison with analytical solution of the response of a homogeneous and isotropic water-saturated poroelastic finite column under harmonic load is presented. The results illustrate the capability this finite element approach to reproduce accurately the response of quasi-static phenomena in a saturated porous media.

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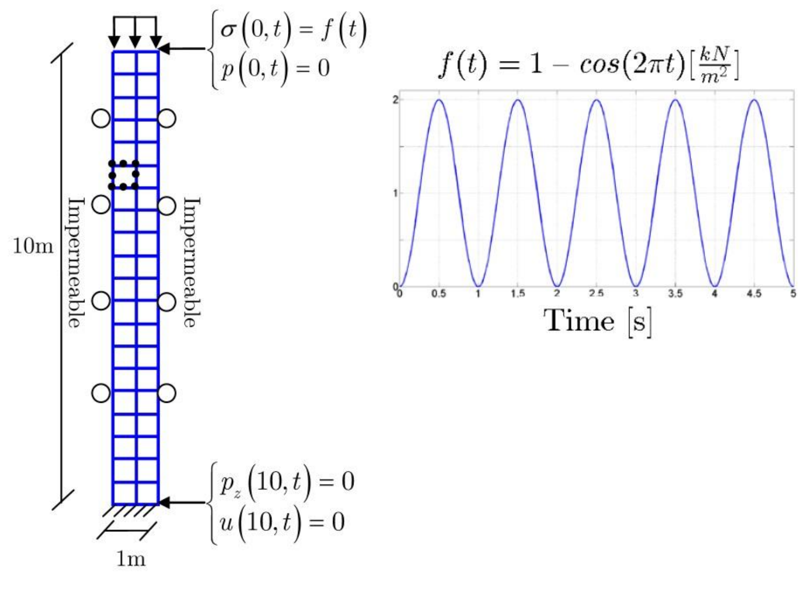

Figure 1 : *Geometry, boundary conditions, mesh and loading path for the numerical simulation.*

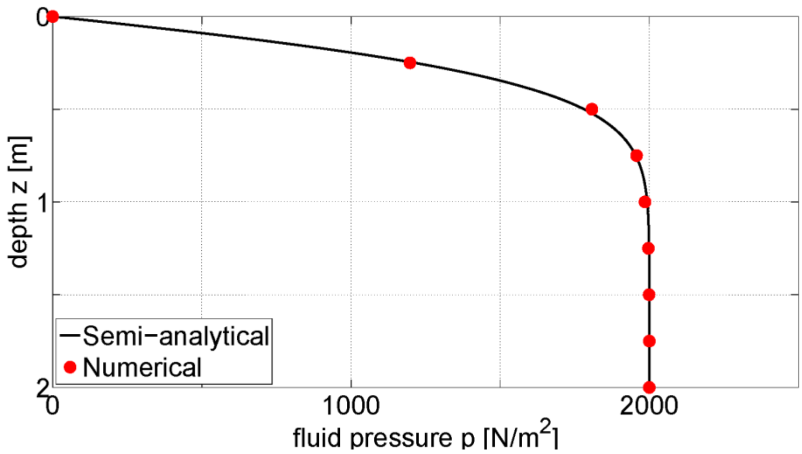

Figure 2 : *Numerical versus semi-analytical pore pressure distribution with depth at t=0.5s for $k=10^{-4}m/s$.*

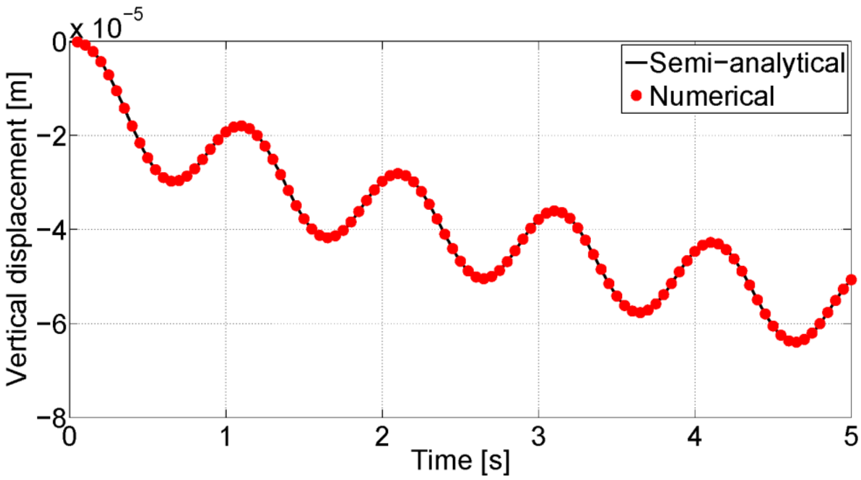

Figure 3 : *Numerical versus semi-analytical vertical displacement at the top boundary for $k=10^{-4}m/s$.*

Enabling Accurate Condition Monitoring with Embedded Nanoparticle Sensing

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Keywords: Molybdenum compounds, Elastico-Mechano-Luminescence, Condition-monitoring.

Abstract:

Elastico-mechano-luminescent (EML) properties of Europium-doped Molybdenum Aluminate ($MoAl_2O_3$:Eu) were trialed as a method to identify position and magnitude of localised high-stress component values and discrete material damage in a pseudorock sample subjected to uniaxial compression. The deformed pseudorock sample is translucent and is used to represent a geomaterial mimic, with the EML emission generated in response to dynamic loading of the embedded nanoparticle sensors.

This work aims to generate an enhanced understanding of rock deformation by providing intra-sample measurements of the influence of rock behaviour and the multi-factorial conditions that lead to rock deformation, particularly to fracture, fluid flow and changes in temperature distributions. This would represent a step change from current practices of post-failure analysis, without any direct intra-sample measurements, and "best-fit" modelling to provide a deeper understanding of rock properties and the state of the potentially multi-phase fluids that they contain. Typically, such experiments collect sparsely distributed data, often collated from post-experiment analysis or in real time via external sensing methods (1-4).

Within this research, $MoAl_2O_3$:Eu EML nanoparticles were incorporated within an epoxy thermoset resin with mechanical properties analogous to rocks. A mixing ratio of 1:200 nanoparticle/resin (by weight) has been found to yield optimal emission, while retaining sample translucence, and a 1:5 mixing ratio yields maximum emission with a reduction in translucence. The inclusion of the EML nanoparticles within the epoxy resin significantly alters the mechanical properties of the sample, with the lowest nanoparticle ratio (0.5% by weight) producing a brittle sample prone to rapid failure/fragmentation. The highest nanoparticle ratio (20% by weight) exhibits higher yield strain with little or no sign of brittle fracture, more representative of sandstone (geomaterial) under triaxial load.

This work introduces nanoparticle sensing and expands on the potential of EML for pseudorock deformation monitoring. A summary of the fabrication process and experimental procedure used to observe the stress conditions within a luminescent nanoparticle-polymer

resin mixture under uniaxial load conditions are also presented. Emission spectra for $MoAl_2O_3$:Eu samples mixed at 20% by weight are presented, with emission peaks consistently observed at ~520 nm for a uniaxial load up to 4.9 MPa (Figure 1). These results indicate that EML nanoparticle-polymer resin compounds act as useful analogues for studying dynamic and quasi-static behaviour in rocks.

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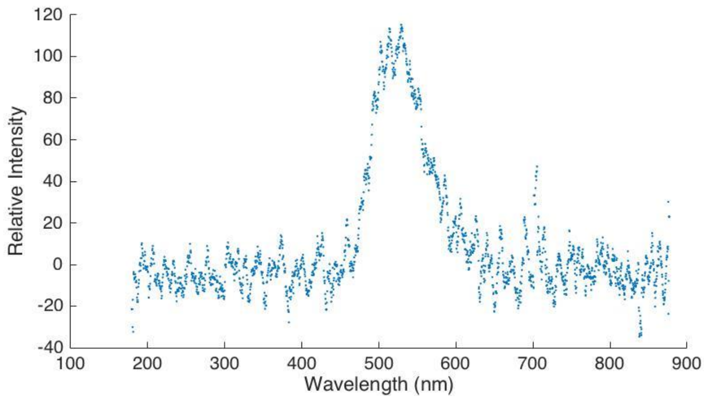

Figure 1: *Mechano-luminescent emission spectrum of Europium-doped Molybdenum Aluminate (Sample 2)*

Viscoplastic rheological model for rock avalanches

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Keywords: constitutive modeling, viscoplasticity, rheology, avalaches, landslides

Abstract

Rock avalanches, at large scale, behave as fluidized granular materials. At small scales we can observe phenomena such as inverse grading and crushing of rock blocks, which results on a change of granulometry and of dilatance properties.

The behaviour of this granular fluid can be modelled using either discrete element methods or continuum based rheological models. The former presents the advantage of reproducing in a natural manner crushing and inverse grading phenomena, but the computational cost of modelling a real avalanche is still difficult to afford.

On the other hand, the latter reduces the cost, but suitable models have to be used to describe the constitutive/rheological behaviour of the granular fluid.

And it is because of this fluid like behaviour that rheological models have been used traditionally to model rock avalanches, as in other types of avalanches.

While mudflows, lahars, and some cases of debris flows have been approximated using models such as Bingham, rock avalanches present a dominant frictional behaviour requiring a different approach.

In his pioneering work, Bagnold (1954), performed tests on a new rheometer able to control inner pressure and volume, and proposed a simple model. Bagnold model included simple shear and pressure terms which depended on the shear strain rate γ (dispersive stresses). The shear stress was given by the law

$$\tau = \mu\gamma^2 \tag{3.1}$$

where μ is a material constant.

This is a particular form of the generalized viscoplastic fluid proposed by Chen (1988)

$$\tau = s + \mu\gamma^m \tag{3.2}$$

where s characterizes the material strength (cohesive-frictional), and m is a material constant.

From here, there exist two alternatives, which depend on the mathematical model being used:

(i) Use these laws in simple shear infinite landslide models which allow to relate the depth averaged velocity of the flow and the basal shear stress, implementing the in depth averaged codes.

(ii) Generalize to 3D the laws obtained in simple shear rheometers and implement them in 3D finite element or SPH codes.

The first approach will be used in this work, comparing the results obtained with different rheological models in real cases.

One possible alternative has been shown to use viscoplasticity of Perzyna type, because it can provide suitable laws both for the solid and the fluidized behaviours, as shown in (Pastor et al 2013, Pastor et al 2014). One most interesting conclusion is that from Perzyna's viscoplasticity, it is possible to derive simple rheological laws which can be used for frictional fluids.

Here, we have considered three rheological laws, which can be applied to model frictional fluids:

(i) Voellmy law, (ii) the viscous frictional law and (iii) the viscoplastic Perzyna based law

These laws have been implemented in a SPH depth integrated code, and they have been applied to Thurwieser rock avalanches to compare the influence of the rheology on the avalanche properties (Manzanal et al. 2016).

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Figures

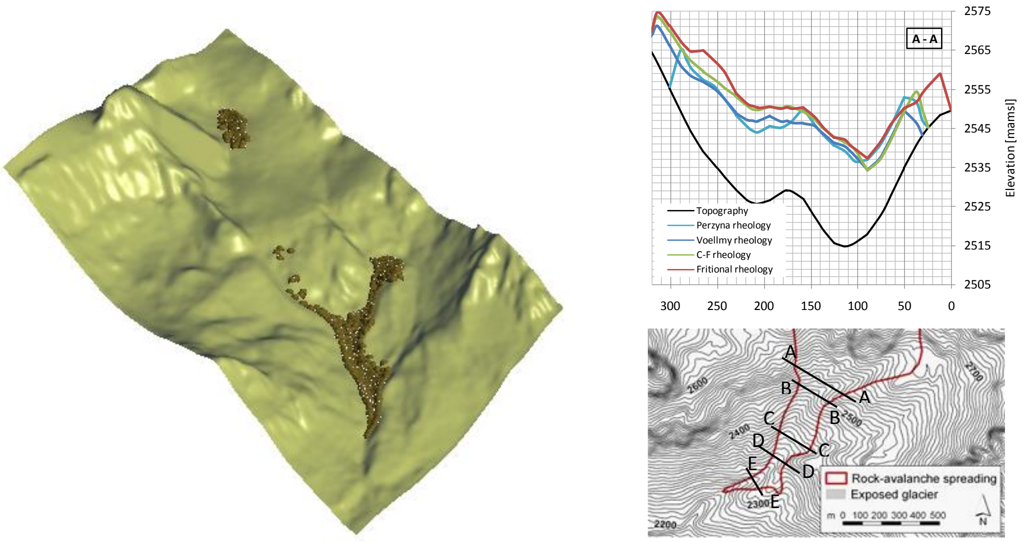

Figure 1 : *Thurwieser avalanche: comparison of cross section for different rheological models and the propagation in 3D terrain for 90s for Perzyna rheological model.*

A two phase SPH model for debris flow propagation

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Keywords: Debris flow, SPH, Fast landslide propagation, Two-phase SPH mathematical model.

Abstract:

This poster presents a model which can be used a particular type of fast landslides, where the coupling between solid and pore fluid plays a fundamental role. The approach is based on the mathematical model proposed by Zienkiewicz and Shiomi (1984), which is similar to those of Le and Pitman (2005) and Pudasaini (2012). The novelty is the numerical technique used, the Smoothed particle Hydrodynamics (SPH). We propose to use a double set of nodes for soil and water phases, the interaction between them been described by a suitable drag law. It is interesting to note that this model allows the use or a more realistic friction angles for the solid phase.

The model is applied to a simple case where shocks and expansion waves appear.

Debris flows is the more complex phenomenon from the modelling point of view, as both solid particles and water can have different velocities. The models have to include velocities of both solid and fluid phases, and the stresses acting on them.

In a previous publication, the authors have addressed the problem of coupling SPH with a series of finite difference meshes associated to each SPH node, which provides better accuracy to reproduce pore pressure changes Pastor et al (2015b). Here, we will model debris flows using two sets of nodes, describing the water and the solid phases, which can move relative to each other.

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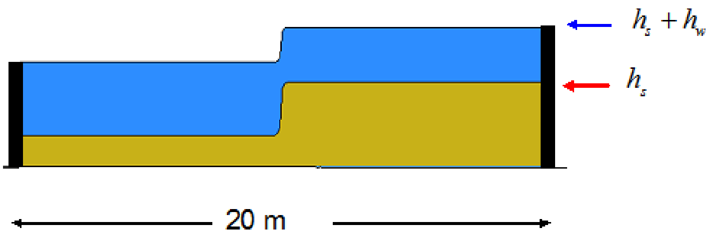

$\rho_s = 2000\, Kg / m^3$

$\rho_w = 1000\, Kg / m^3$

$n_L = 0.69$

$n_R = 0.39$

$\tan\phi = 0.0$

Interaction law (Anderson)

$R = -nR_w = (1-n)R_s$

$R = C_d\left(v_w - v_s\right)$

$$C_d = \frac{n(1-n)}{V_T n^m}(\rho_s - \rho_w)g$$

$V_T = 1.0e-3$

$m = 1$

Figure 1 : *Shocks and expansion waves*

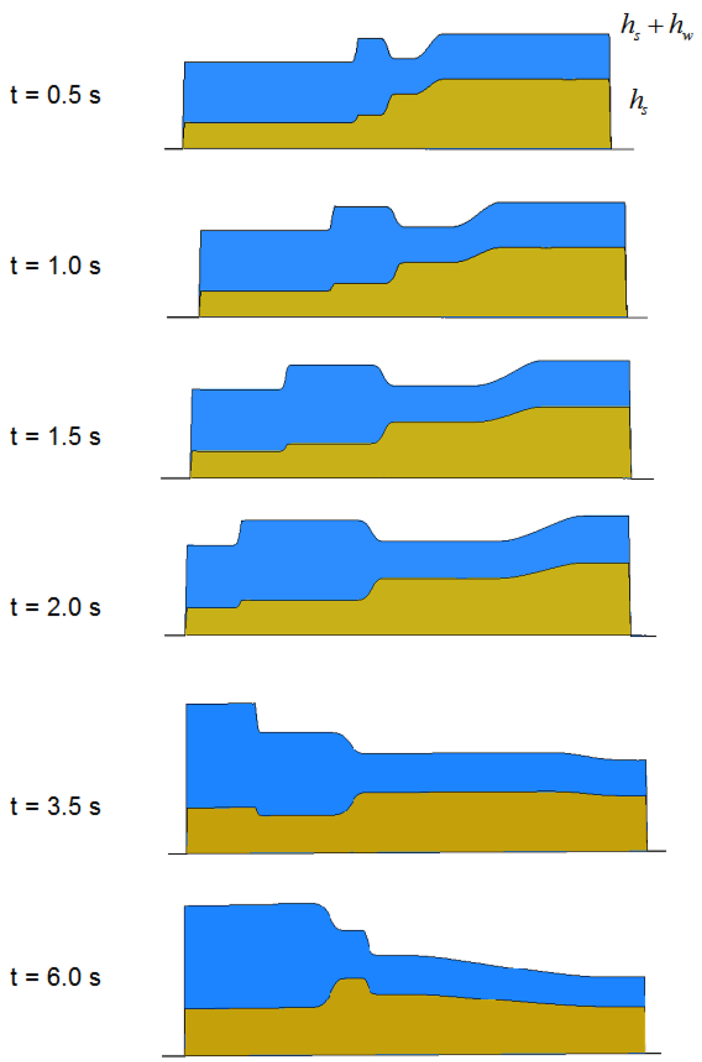

Figure 2 : *Profiles of* h_s *and* $h_s + h_w$ *at times 0.5, 1.0, 1.5, 2.0, 3.5 and 6 s*

SPH-FDM propagation and pore water pressure modelling for debris flows in flume test

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Keywords: debris flow, flume tests, SPH, FDM, pore water pressure, propagation, rack.

Abstract

Debris flows are dangerous phenomena due to their large run-out distances and high velocities. The time-space evolution of the interstitial pore water pressures much affects the propagation stage of debris flows.

This work provides a contribution to this topic through the use of an enhanced numerical model, which combines a 3D depth-integrated hydro-mechanical coupled SPH (Smooth Particles Hydrodynamics) model for the propagation analysis and a 1D vertical FDM (Finite Difference Method) model for the evaluation of the pore water pressure along the height of the flowing mass (Pastor et al., 2015). The SPH-FDM model is used to simulate well-documented flume tests performed in USA through a 90 m long channel exiting at a sub-horizontal pad (Iverson, 2003). For these flume tests, they were carried out the simulations with the SPH model proposed by Pastor et al. in 2009 and with the SPH-FDM model (Pastor et al., 2015). This choice was done because the first depth-integrated model solves the SPH propagation equations assuming a quarter cosinus shape function for vertical profile of pore water pressures, while the second model may compute - through a set of finite difference mesh (FDM) - any general vertical profile of pore pressures in relation to the hydraulic boundary applied to the ground surface. Figs. 1 a-b show the comparison between the flume test measurements and the numerical simulation at points A, B (Cascini et al., 2016), for both propagation height and basal pore water pressure. The comparison is presented with reference to t-t_{flow}, where t_{flow} represents the time when the flow reaches the observation point.

The model is later used to simulate other flume tests, performed in Japan in a 3.4 m long channel, equipped without or with a (permeable) rack at the end of the channel, which allows the pore water pressures reducing until the mass eventually stops (Gonda, 2009). The run-out distances measured are compared to the numerical simulations in Fig. 2 (Cascini et al., 2016). The figures show that the SPH-FDM model is capable to properly reproduce the time-space evolution of the pore water pressures during the propagation stage with different geometries of experimental flumes and different hydraulic boundary conditions.

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Figures

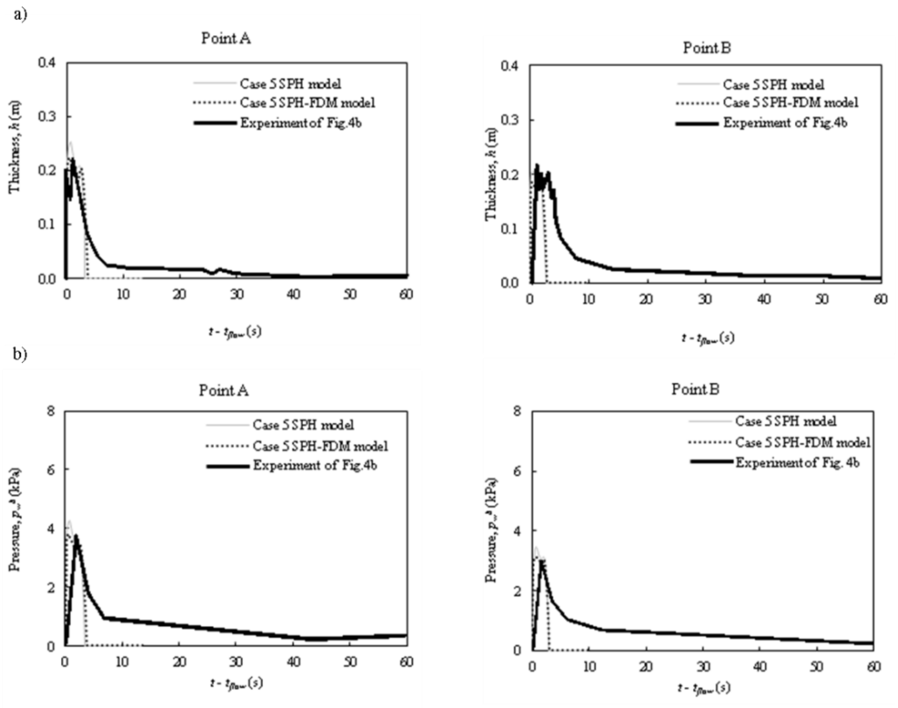

Figure 1 : Comparison of the flume test measurements and numerical simulations: a) evolution of flow depth (*h*); and b) evolution of basal pore water pressure (p^b_w) at the points A and B. The legend refers to the experiment of Fig. 4b and the numerical simulation of the Case 5 of Table 2 shown in the paper Cascini et al. (2016)

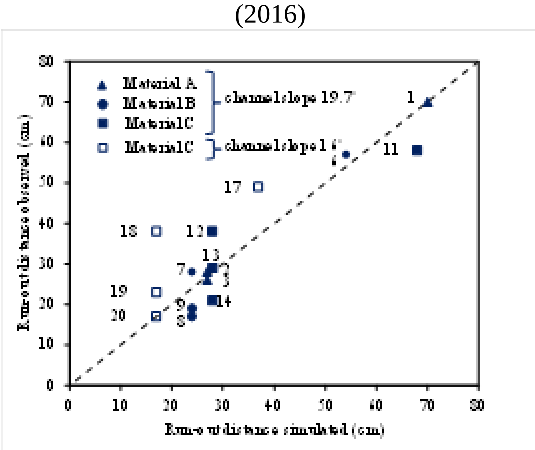

Figure 2 : Comparison of the experimental measurements and the numerical simulations of the run-out distances on the rack. The legend refers to the different material and channel slope and the numbers represent the experimental conditions of the Table 3 in the paper of Cascini et al. (2016).

Stochastic heterogeneous material modeling for wave propagation in a ballast layer

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Abstract

The dynamical behavior of granular materials gives rises to interesting behaviors on large distances. The discrete nature of the material and the complex interaction between the grains produce a "non trivial" mechanical behavior. Experimental set-ups shows the presence of a dispersion behavior in pre-stressed glass packing [4]. The signals were decomposed in a coherent pulse, and a coda consisting of seemingly random multiply-scattered waves. Variations in the coda regions was stressed by the variation in the glass packing size. Another study performed in water tank filled with glass beads, gave us experimental dispersion curves. It presents a clear slow wave, whose velocity is slower than both bulk waves in water and glass [5]. Both phenomena can be explained by the strong heterogeneity of the medium and also appear in other media (as the Earth for example [1,2]), independently of the continuous or discrete character of that medium. On the numerical side, we are looking for models that can reproduce a similar dynamical behavior. Leibeg [3] presented a simple model based on discrete masses linked by springs with random stiffness, which is capable to represent qualitatively the this response. In this work, we propose a stochastic heterogeneous continuum model for granular media. This model can be seen as an extension of the model proposed by Leibeg. The identification of the parameter of that stochastic model is performed with respect to simulations of discrete granular media. Finally, we applied this model to simulate the wave propagation on a ballasted railway track.

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Rock-Bed Thermocline Storage: Numerical Analysis of Granular Bed Behavior and Interaction with Storage Tank

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Keywords: Thermal Energy Storage (TES), thermo-mechanical behavior, thermal ratcheting, granular filler, Discrete Element Method (DEM), numerical simulation

Abstract

1. Introduction

Thermal energy storage (TES) systems are central elements of various types of power plants operated using renewable energy sources. In Concentrated Solar Power (CSP), storage can mitigate the variability and intermittency of solar radiation and allow for a continuous operation. Packed bed TES can be considered as a cost–effective solution for such applications. It offers a direct contact between the heat transfer fluid and solid matrix and an additional freedom for the choice of the storage materials, thus a further reduction in the inventory's cost.

However, such designs might experience structural failure, due to a phenomenon known as thermal ratcheting. The premature tank failure is provoked by an excess of thermal stresses accumulated during cycles. As an example, when rock are used as storage material, the tank wall expands more than the solid medium during charge process, a gap is created between rocks and tank walls and the filler material is settled down to fill it. During discharge, the tank contracts against the bed, resulting in thermal stresses that may exceed the wall tank yield stress and generate plastic deformation. This phenomenon is repeated over the cycles and the tank will be slowly ratcheted outward until it fails. Up to now, the significance of this phenomenon is not well understood and has to be studied as it strongly impacts tank design and life-time.

2. Numerical models for thermal ratcheting simulation

Two approaches are usually considered to model the thermo-mechanical behavior of packed beds in storage tanks. The first approach lies on considering the packed bed as a continuum media by assuming that its microstructure is small compared to the containment size. Homogeneous and isotropic properties have to be attributed to the filler material, and the stochastic character of such randomly arranged particles is neglected, thus the densification of the filler cannot be well reproduced.

Most of works that used this approach are based on the experimental structural response of the 170 MWh thermocline tank integrated in the Solar One pilot plant [1, 2]. However, these experimental data suffer of large uncertainty which limit the capability of understanding the thermo-mechanical behavior of the packed bed [3]. In addition, the tank was no more functional after only few cycles, reducing the possible effects of thermal ratcheting on the tank.

In contrast, a more detailed model approach, called 'discrete element method' (DEM) and based on the macroscopic behavior of the filler can be considered. In DEM approach, the discontinuous nature of granular materials is represented by a set of discrete rigid elements and the forces between interacting particles and walls are computed based on a friction-spring-damper system defined at the contact locations; the resulting displacements are determined by integrating Newton's second law.

Only few studies were performed using DEM approach. Dreißigacker et al. [4] used DEM to study the thermo-mechanical behavior of a spheres packed bed. The simulated results were compared with experimental data from a test rig consisted of 0.9 m^3 of filling volume in a quadratic cross-section tank. The containment walls are considered as fixed walls. The calculated and measured results show a satisfying agreement.

3. Thermo-mechanical study

For getting a better understanding of packed bed behavior and its interaction with tank walls during successive thermal cycling, a new model is developed based on the DEM. The mechanical model is coupled to the thermal expansion of particles via Equation 1, where d is the diameter particle and α_b is the linear expansion coefficient of the packed bed. The expansion of spherical particles is proportional to the differential temperature at position z.

$$d(z) = d_0(z)\,[1 + \alpha_b(T - T_0)(z)] \qquad \text{(Eq. 1)}$$

The calculation procedure consists of firstly determining the particle size, then computing the interacting recoil, friction and damping forces followed by computing the resulting particle displacement by integrating the second law of motion.

The simulations are performed using the open-source code YADE [5]. Mechanical and thermal properties of the filler material have been experimentally determined by performing loading and unloading tests on a representative elementary volume of the filler. Experimental temperature profiles used for thermal loads are obtained from the rock-bed thermocline STONE set-up [6].

The study, for which an illustration of its geometry is represented in Fig. 1, was initially focused on fixed tank walls as most of existent studies using DEM approach. Results show that, when considering fixed walls, wall stresses are more important in charge than in discharge. This result is contrary to what is experimentally observed in rock-bed thermocline TES, indicating that the classical "fixed walls" assumption is not valid. Then, movable walls are considered to investigate the real mechanisms that take place in thermocline-like storage tanks.

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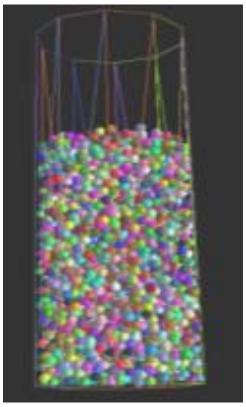

Figure 2 *: Schematic representation of the geometry using DEM approach*

DEM-LES simulation of sediment transport initiation

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Keywords: Discrete Element Method, DEM, sediment transport, grain-scale, turbulence, LES, IBM, bedload.

Abstract

Sediment transport is a pervasive phenomenon and, due to its complexity, a poorly understood one. The initiation of the transport process is in general a function of the characteristics of the sediment bed, and of its interaction with the flow. In particular, the turbulent structures created around the single grains seem to be of great importance for determining the pressure fluctuations necessary for triggering the process. This picture is often overly simplified by the empirical solutions used in engineering practice, highlighting a gap in our understanding of the process. While it is clear that grains-scale approaches cannot be used directly for the solution of engineering problems, they can play an important role in filling this gap. In this work, a new framework for the simulation of transport phenomena is presented. The sediments are idealized as spherical grains, whose mechanics is solved using the Discrete Element Method (DEM). The majority of the grains constitute a rough fixed bed. The remaining ones are freely advected by a gravity-driven current. As a resolution of the full 3D turbulent field is necessary, the current is solved using a Large Eddy Simulation (LES). An Immersed Boundary Method (IBM) guarantees an efficient and stable coupling between fluid and grain motion (see Figure 1). The preliminary results aim at replicating the Shields law for the prediction of transport initiation, and at linking the lift forces experienced by the grains to the pressure fluctuations determined by the surrounding geometry.

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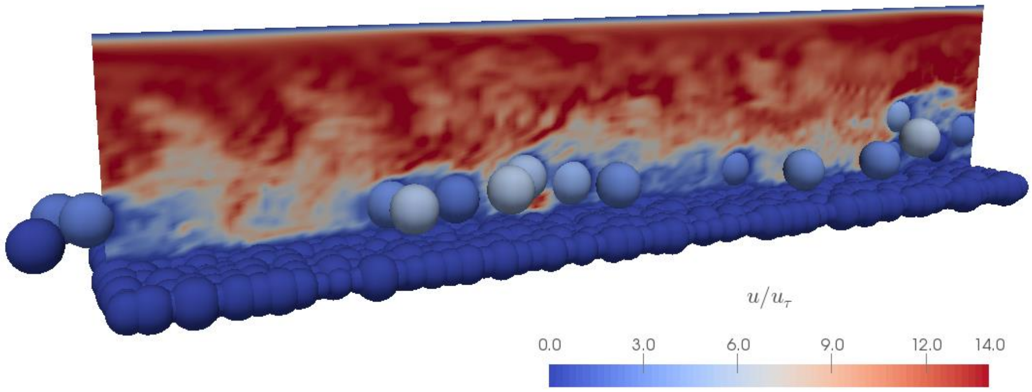

Figure 1: *Instantaneous velocity field, particles and fluid.*

A methodology for the study of foundations for marine structures

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Keywords: Breakwater, Caisson, Finite Elements, Volume of Fluid, Generalized Plasticity

Abstract

A methodology for the study of marine foundations is presented. The response in displacements, stresses and pore water pressures is obtained from a finite element coupled formulation. Loads due to wave action on the foundation are obtained from the IHFOAM model that solves the three-dimensional Reynolds Averaged Navier-Stokes (RANS) equations using a finite volume discretization and the volume of fluid (VOF) method. Additionally, the methodology includes a State Parameter Generalized Plasticity based constitutive model for granular materials capable of representing liquefaction fenomena of sands subjected to cyclic loading, such as those frequently appearing in the problems studied. This methodology is applied to the study of the response of a caisson breakwater foundation.

Geometric and kinematic single grain characteristics observed during triaxial testing of granular materials

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Keywords: Particle shape characterisation, x-ray micro-tomography, digital image correlation.

Abstract

It has been extensively shown in literature that particle shape has an influence on geotechnical properties. It strongly affects both micro and macro-mechanical properties but it is still very difficult to quantify and measure.

Since the early 1900’s, several authors tried to characterise the grain shape and to understand its influence on the overall soil behaviour. Among the most important, Wadell (1932) introduced the concept of “sphericity” that quantifies how a particle differs from a sphere, in terms of surface area. Krumbain (1941) created the first chart to visually estimate shape from the grain length ratios ("flatness" and "elongation" indices). Barret (1980) defined shape as the combination of three independent aspects in function of the scale at which they are evaluated: *form*, measured at large scale and related to sphericity, *roundness*, which is more sensible to the grain corners, and *surface texture*, measured at small scale.

In the recent years, the increasing of computer performances is introducing new ways to study the shape of particles. In particular, image analysis techniques are replacing measurements made by hands or eyes, which are not objective.

Furthermore, due to the difficulty to acquire and analyse images of soil particles in three dimensions, the previous studies are based on 2D measurements. But in order to fully characterise the grain shape, it is necessary to define 3D shape descriptors, which are able to take into account the tri-dimensional nature of particles.

The poster describes first results from an ongoing effort to systematically exploit high quality 3D images of soil particles obtained using x-rays tomographic inspection of triaxial soil specimens performed at 3SR laboratory in Grenoble (Andò et al., 2013).

Two different soils are studied: Caicos and Hostun sands. The specimens, containing about sixty/seventy thousands of grains, are scanned with a resolution of 15.56μm/pixel size. Then, the gray-scale images can be binarised, segmented and finally labelled through image processes (Andò et al., 2013). After this procedure, every grain can be extracted from the specimen (Figure 1) and numerically studied in three-dimensions in order to calculate firstly its geometry (i.e. volume, surface area, lengths, inertia properties) and then its 3-D shape descriptors.

Thus geometric descriptors of a statistical nature can be obtained, some (such as grain size distribution, Figure 2) that have been also traditionally obtained by other means, and others

(such as distributions of different 3D shape parameters) for which much less previous data had been obtained.

Furthermore, geometric -i.e. single scan- descriptors can be usefully complemented by kinematic -i.e. multiple scan- descriptors of the acquired database. The X-rays tomography is a non-destructive procedure that is performed several times during the execution of a triaxial test (about 15 scans per test), allowing step by step tracking of individual particle positions. Making use of the digital image correlation (Software TomoWarp2, developed by S. Hall, E. Andò, E. Tudisco) it is possible to follow every grain during the deviatoric load and to obtain displacements and rotations for all the particles within the specimen. The discrete nature of TomoWarp2 and its parallel algorithm allow to correlate two 3D images in a reasonable calculation time, so that every grain can be followed until the end of the test (Figure 3). The images are correlated in an incremental way, it means TomoWarp2 always tries to correlate the first image (performed at the beginning of the test, called “01”) with the image scanned at the desired step (i.e. “02” or “03” or “04”, etc.). The advantage of doing so is that a single grain can be tracked from the first to the last load step, without being lost. The result of this effort are statistical distributions of kinematic descriptors of single particle motion during the test.

Future developments will use data-mining algorithms to systematically explore the relation between the two databases thus formed. The final goal is to use the empirical relations thus obtained as a cornerstone in the calibration of advanced contact-models for DEM applications in geomechanics.

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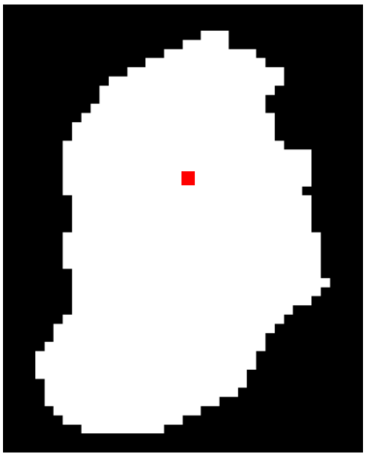

Figure 3: *Slice of a 3-D reconstructed grain.*
The size of each pixel (red window) is 15.56μm and the grain total volume is made up of about 30.000 voxels.

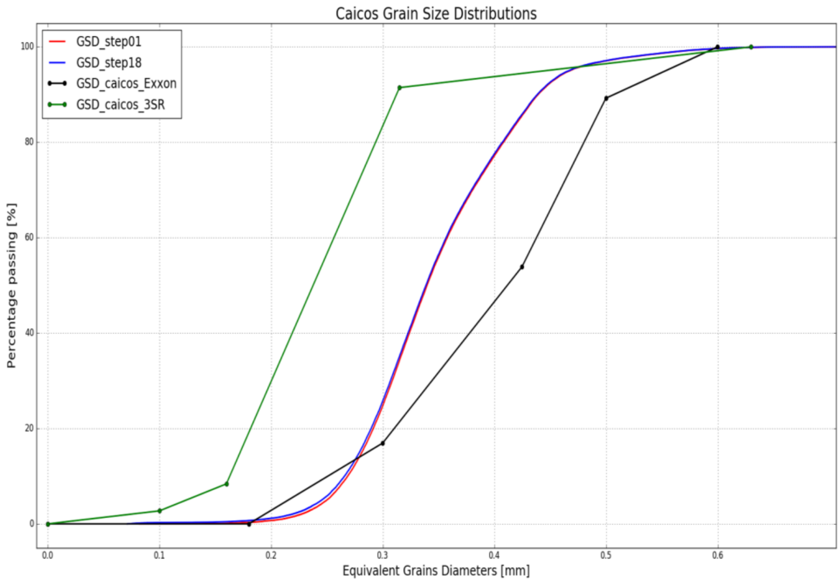

Figure 4: *Grain Size Distribution comparison between sieve analysis (GSD_caicos_Exxon, GSD_caicos_3SR) and image analysis (GSD_step01, GSD_step18)*

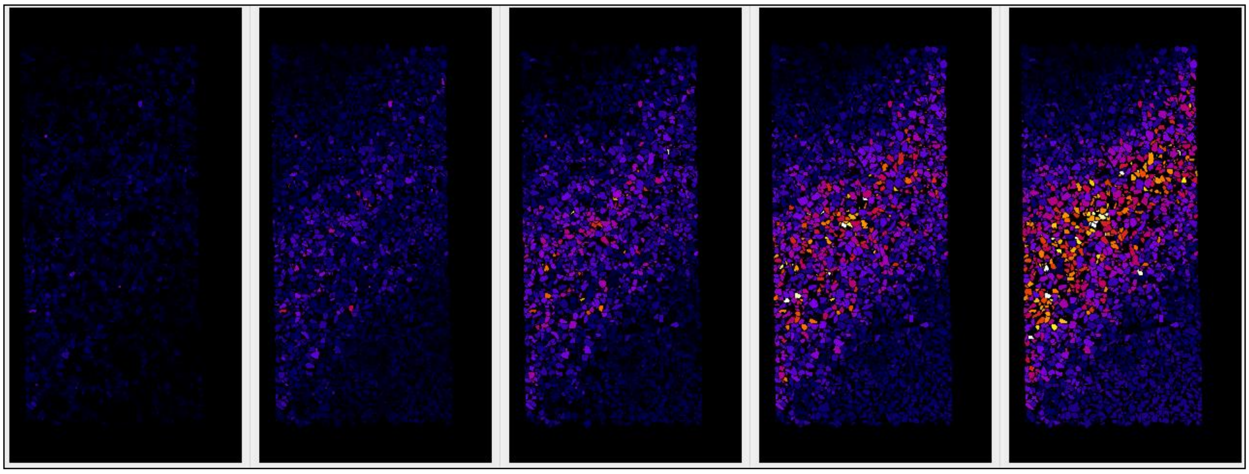

Figure 5: *Vertical slices of Hostun sand specimen showing grain rotation measured over increments during the test. Grains are coloured by the value of their measured total rotation. Not all increments of the test are shown.*

On some numerical issues in non-isothermal multiphase porous media modelling using the finite element method

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Keywords: Locking, Taylor-Hoods finite element, Multiphase porous media models, Mass conservative schemes

Abstract

When modelling multiphase porous materials with the finite element method, some numerical problems may occur. It is the case of locking phenomena due to incompressibility of the medium, e.g. in undrained conditions typical of low permeability materials (i) and the excessive mass balance error when modelling porous media in partially saturated conditions (ii). This work aims to recall the above mentioned problems and to show a possible solution applied to the multiphase porous media model [1].

(i) When mass balance equation and equilibrium equations that govern the behaviour of a saturated porous media are discretized in space (FEM) and time (Euler scheme), the following linear system of equation can be obtained [2]:

$$\begin{bmatrix} \theta \boldsymbol{K}_T & -\theta \mathbf{Q} \\ \mathbf{Q}^T & \mathbf{S} + \Delta t \theta \mathbf{H} \end{bmatrix}_{n+\theta} \begin{Bmatrix} \bar{\mathbf{u}} \\ \mathbf{p} \end{Bmatrix}_{n+1} = \boldsymbol{f}$$

where **S** is the compressibility matrix and **H** is the permeability matrix. If the incompressibility of solid grains is assumed and the permeability matrix **H** tends to zero for low values of the permeability, then the numerical locking occurs; the use of finite elements with $n° \, dof_{,u} \geq n° \, dof_{,p}$ that pass the simple patch test solve the problem (i), as described in [2].
In this framework, a case study of a column of a poroelastic saturated material subjected to a harmonic load has been studied and the finite element solution has been compared with the analytical solution. The numerical solution has been obtained with the Taylor-Hood finite element (Q8P4), and the standard bi-quadratic element (Q8P8) using two different values of permeability ($k = 10^{-5}$ m/s and $k = 10^{-13}$ m/s).
The results plotted in *Figure 1* show that the standard Q8P8 elements, although showing very good results with the highest value of permeability, leads to large oscillations and meaningless results with the lowest value of permeability, while the Taylor-Hood Q8P4 is stable also in undrained conditions.

(ii) When partially saturated porous media are modelled using FEM the computation of the time derivative of the water saturation plays a crucial role. If standard chain rule is applied (in order to move the derivative on water pressure, e.g. [1]) excessive mass balance errors can occur, due to the non-linearity of the saturation-capillary pressure curve. To solve this problem, a direct numerical discretization of the time derivative of the water saturation can be adopted [2].
The desaturation of a soil column initially saturated with liquid water, the Liakopoulos test (*Figure 2*), has been studied using a FEM formulation in which both the two above mentioned time discretization have been implemented. The solid skeleton is considered rigid, similarly with the simulations presented in [3]. The results plotted in *Figure 3* show the relative mass balance errors in the two cases, with very high value when using the chain rule, which is, in this case, limited to the first part of the desaturation process.

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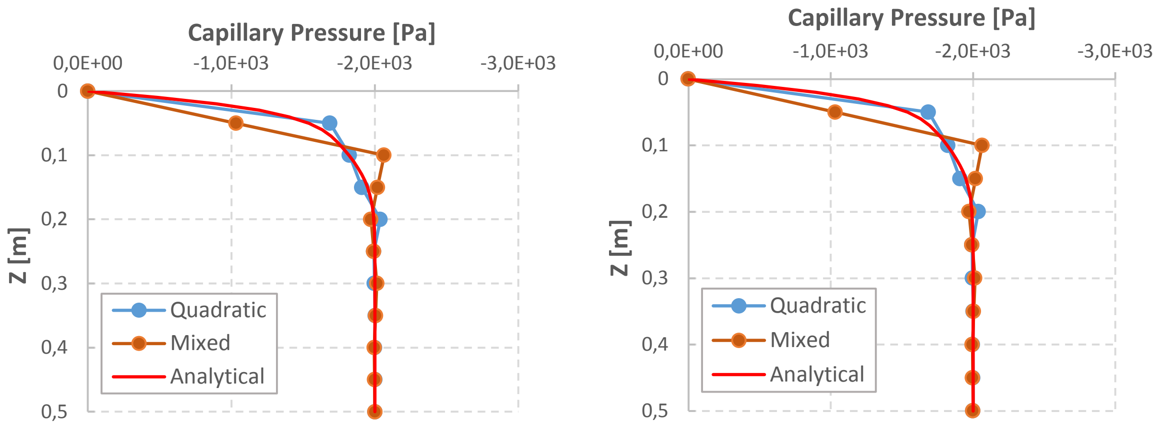

Figure 1 : *Water pressure distribution along the height of the column for k = 10^{-5} m/s (left) and k = 10^{-13} m/s (right), at t = 0,15 s.*

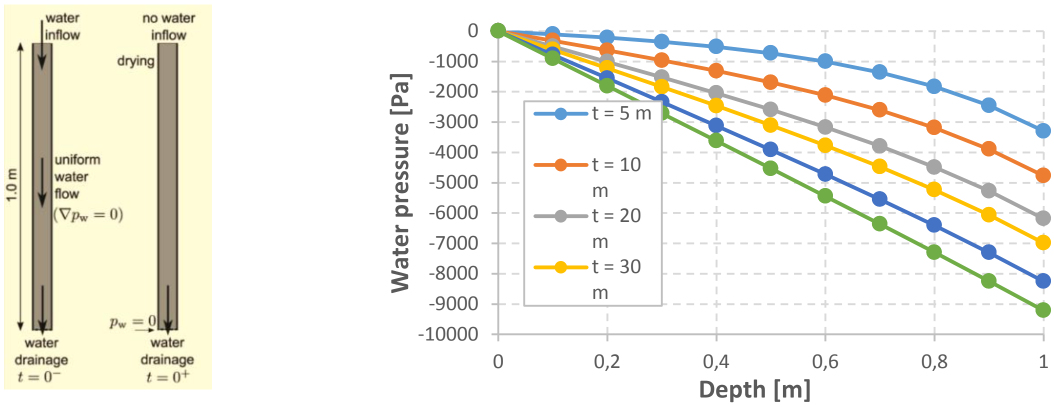

Figure 2 : *I.C. and B.C of Liakopoulos experiment (left) and negative pore pressure evolution in time (right).*

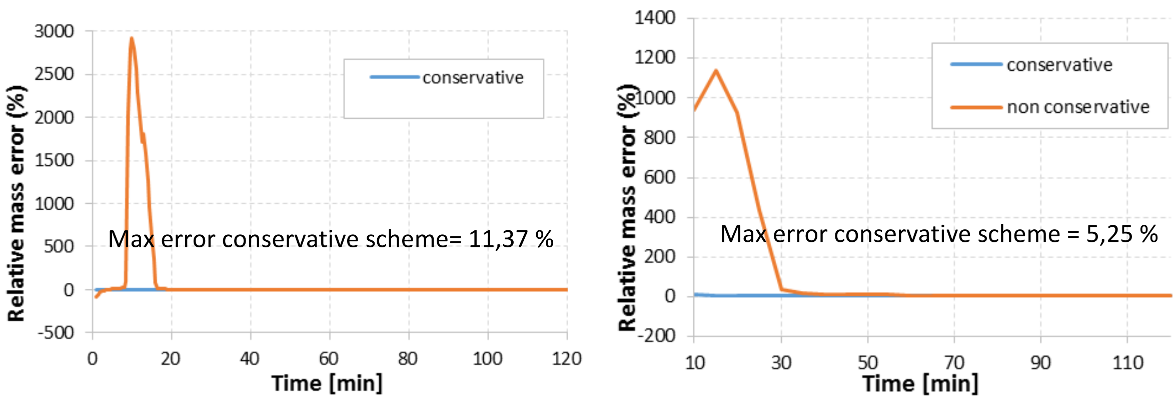

Figure 3 : *Mass balance errors comparison using two different time stepping: Δt = 5 min (left) and Δt = 30 s (right).*

Deformable porous media saturated by three immiscible fluids: Constitutive modeling and core flooding simulations

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Keywords: Immiscible fluids; Capillary pressures; Relative permeabilities; Core flooding

Abstract

A number of enhanced, or tertiary, hydrocarbon recovery processes, such as gas or steam injection and water alternating gas injection, require three-phase modeling, as they involve the co-existence of three immiscible fluids, typically water, oil and a gas. The relative wettability of the three fluids is known to influence significantly the macroscopic properties that govern multi-phase flow, like capillary pressures and relative permeabilities. Thus, understanding formation wettability is an important aspect in optimizing oil recovery.

In a water-wet rock, water is more wetting than oil which is more wetting than gas. The contact angle between water and oil is smaller than 90°, oil is spreading spontaneously, and water keeps preferentially in contact with the rock matrix. Consequently, small pores contain mostly water, oil may invade intermediate and large pores and gas is restricted to the middle of large pores. This configuration motivates the water-oil capillary pressure $p_{oil} - p_{water}$ to be a function of the sole oil saturation and the oil-gas capillary pressure $p_{gas} - p_{oil}$ to be a function of the sole gas saturation, e.g. see Helland and Skjæveland~[2004],

$$p_{oil} - p_{water} = p_{cow}(\underline{S}_{oil}), \quad p_{gas} - p_{oil} = p_{cgo}(\underline{S}_{water}) \qquad (1)$$

In a three-phase context, the above expressions need to be upgraded, in particular to meet certain consistency conditions along the edges of the saturation. Moreover eqn (1) refers to effective saturations which account for the irreducible saturations. The problem of conceiving a general definition for effective saturations is not a trivial task in the presence of three immiscible fluids.

The order of wettability has quantitative consequences also on relative permeabilities. In fact, the relative permeability to water is larger for oil-wet systems than for water-wet systems, and the opposite applies to the relative permeability to oil.

The following ingredients are worked out:

1) simple, although general and original, formulas for the effective saturations;
2) constitutive expressions for the three relative permeabilities of water, oil and gas in terms of effective saturations;
3) constitutive expressions for the capillary pressures;
4) a time marching scheme including lumping of the storage contributions.

The above items are implemented in a domestic finite element code, considering the solid displacement vector and the three fluid pressures as primary variables.
Gas injection, water alternated gas injection tests and co- and counter-current imbibition tests are simulated as a check of the reliability of the constitutive and computational framework.

Revisiting scan line void fabric definitions using DEM

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Keywords: Void fabric, Scan line, DEM

Abstract

An important and possibly key feature to the soil behavior that has been taken only lately into account is the fabric. Fabric and its elements seem to be important for the mechanical response of soils. In this vein, many researchers in the last decades have tried to introduce the fabric as an extra variable in a soil constitutive model. The types of soil fabric used in constitutive modelling are related to different microstructural entities such as particle long axis orientations, inter-particle contact normal directions (e.g Oda et al. 1985), or orientations of void shapes expressed by properly defined void vectors; in the latter case they can be succinctly called void fabric tensors (e.g. Ghedia & O'Sullivan 2012).

Several methods have been proposed in order to measure the fabric with respect to the voids (e.g. Li & Li 2009; Oda et al., 1985); nevertheless there is not much research on the relations between void and solid fabric. Void fabric is of particular interest since graphical approaches are well defined experimentally, some of them can be also applied in numerical experiments, like the scan line method, while contact normal vectors are difficult to determine for natural granular materials, due to problems associated with accurate measurement of tangent contact planes (Jaquet, Andó, Viggiani & Talbot, 2013).

In the current work, the authors discuss the application of the "graphical" method where voids are quantified by a method based on the parallel scan-line approach of Oda et al (1985) based on significant micromechanical and macromechanical observations and reasoning. The authors performed several computational tests using DEM to evaluate the "graphical method" and existing well established definitions on void fabric described above. In particular, PFC 2D is used to evaluate the scan line method defined by Oda et al (1985). It can be observed that existing "graphical" scan-line definitions applied to images do not provide compatible results with analytical measurements obtained from computational tests; the validation procedure includes several options and "virtual" experiments.

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Impact forces of dry granular masses on rigid barriers: comparison of empirical and theoretical approaches with DEM numerical results

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Keywords: DEM, debris flow, impact forces, rigid barriers

Abstract

In the design of sheltering structures as protection measures for very rapid landslide risk mitigation pseudo-static approaches are very often employed. In this perspective, the authors present the problem of the assessment of the maximum impact forces transmitted by dry granular (non-cohesive) masses (MIF) to rigid barriers, using DEM numerical results and provide a formula which defines the dependence of the maximum impact force on the Froude number and a change in the overall behaviour of the soil mass regime (from solid like to fluid like) according to a proper measure of the dynamic material stiffness. It is worth noticing the several different parameters of the soil-barrier system included in the formula which are not yet considered in the existing practice and codes.

Then, the numerical results, obtained by the authors by employing a DEM code, with the data available in the literature, commonly used to assess the value of the maximum impact force transmitted by a sliding dry granular mass to a rigid barrier, are compared. The comparison is not easy, since numerous are the formulas proposed in the literature and numerous are the field and the experimental data obtained by performing small scale tests. To simplify the analysis, the numerical data obtained by the authors were compared separately with Hydrostatic (HS), Hydrodynamic (HD) and Boulder Impact (BI) approaches.

The approach proposed by the authors is thus employed to (i) discuss the reliability of the existing practice procedures, (ii) highlight the reasons of the scatter among the values obtained by using the approaches proposed in the literature, based on hydrostatic, hydrodynamic and boulder impact theories, (iii) underline that the empirical formulas available in the literature do not take into consideration a series of factors, like, for instance, the front inclination and the void ratio, that in contrast severely affect the maximum impact force value.

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Effect of spatial variability on the micromechanics of sand

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Keywords: Spatial variability, model test, triaxial test.

Abstract

Even though increasingly sophisticated models are proposed in order to faithfully reproduce topology, spatial distribution and thickness of strain localization patterns in sand (e.g. Cosserat continuum, second gradient regularization, etc.), the particulate nature of the material is often disregarded by considering a homogeneous continuum in the framework of the element test.
Willing to study the influence of porosity spatial variability on the response of granular materials at the particle scale, triaxial compression and extension test are numerically simulated by adopting a simple plasticity model accounting for fabric change and reproducing the initial porosity field measured on real specimens subjected to the same tests into an x-ray scanner.

The good accordance between the experimental and the numerical results reveals spatial variability as a key factor to catch the behavior of granular materials.

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Figures

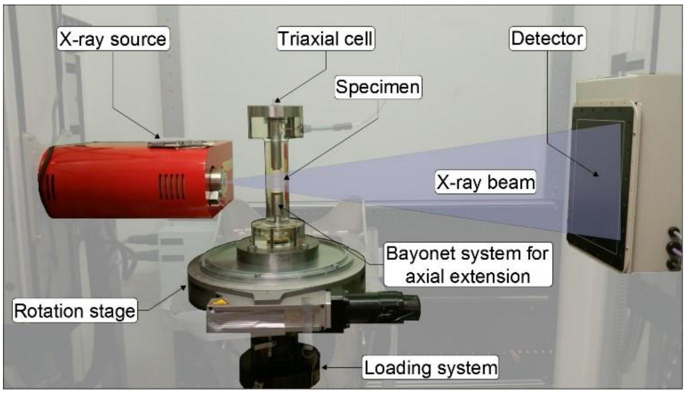

Figure 1: *Setup of the triaxial equipment in the x-ray scanner.*

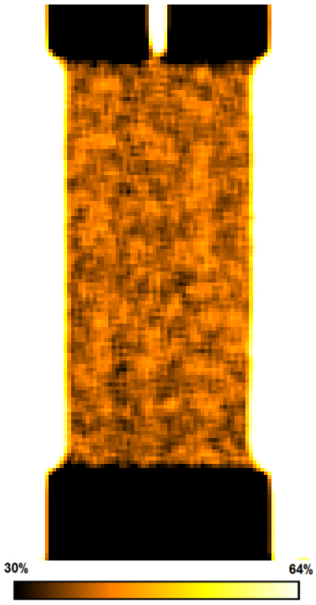

Figure 2*: Measured Porosity map.*

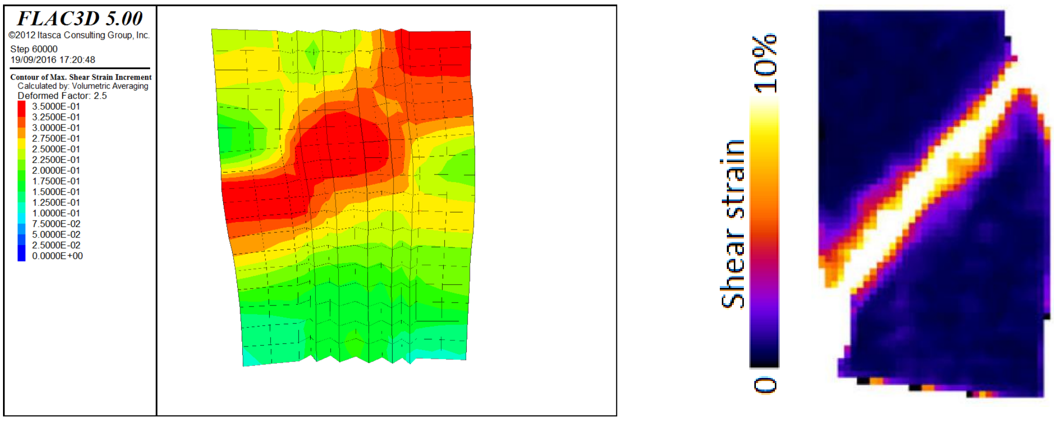

Figure 3: *Comparison between numerical and experimental result.*

Thermo-chemo-mechanics in enhanced geothermal reservoirs

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Keywords: Shear fracture, enhanced geothermal reservoir, fluid-rock interaction, thermo-chemo-plasticity, permeability.

Abstract

Recently, the technique of Enhanced Geothermal System (EGS) has been employed to unlock thermal energy extraction from low permeability reservoirs. The key idea is to increase hydraulic connectivity between a pair of injection and production wells, in order to allow an economic flow rate (e.g. Desert-Peak geothermal field test, Nevada [1]). By pressurizing cold water into deep earth (1000~3000m beneath the ground), generation of new tensile (mode I) cracks as well as reactivation of pre-existing shear (mode II) fractures are achieved, which provides sufficient heat exchange surface area to extract energy from the hot environment. Being initially hot, the rock adjacent to the injection outlet is then subject to cooling-reheating cycles. The effects of acids on mechanical properties of tensile fractures have been modelled [2] and tested [3], while the re-activation of shear fractures under thermal and chemical loads could be treated as an analogy to a transient slip of chemically active faults [4]. Shear localization, indicating potential traces of shear fracturing, is investigated in this study (see Fig. 1).

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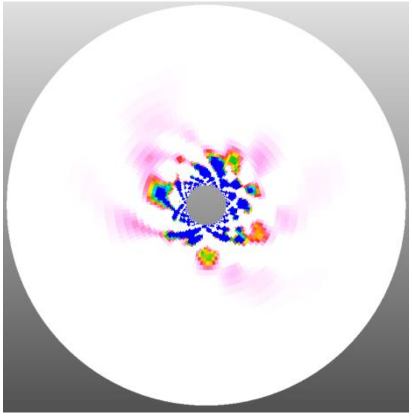

Figure 1: *Shear stress pattern around a borehole.*

Grain breakage under uniaxial compression (3D DEM modelling)

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Keywords: DEM, Grain Breakage, Granular Media, Numerical Model, NSCD

Abstract

Recent studies conducted on rockfill structures have shown that the construction processes rely on empirical methods. Therefore, the stability of this type of structures depends on the methods used to design, execute and compact the structure. A particular property of rockfill is the big grain size, which can lead to important particle breakage when subjected to standard stresses [1], which may then lead to considerable, and sometimes dangerous, settlements. Technological advances still do not offer big enough apparatus, required for experimental studies and characterisation of rockfill materials. For this main reason, numerical approaches are often adopted to characterize these materials, in addition to evaluating the effect of a wide variety of parameters.

The discrete element method (DEM) is the most adapted method to represent this type of discontinuous material, taking into account grain breakage. In our study, in order to simulate grain breakage, we chose this method (DEM), and more specifically the Non-Smooth Contact Dynamics (NSCD) method [2] implemented in the open-source software LMGC90. The NSCD method describes the overall behaviour of a collection of objects by taking into account the dynamics of each element and the interactions between these elements. Two levels are involved in solving the problem: global (kinematic) variables are used to express movement equations of the particles, and local (contact) variables are used to describe the interactions. Many models have been suggested [3,4].

In our study, we present a three-dimensional grain model based on the concept of particles assembly using cohesive bonds. In order to find a model, as close as possible to reality, a script was written to generate a polyhedral grain, by assembling tetrahedral particles and joining them together using cohesive bonds. The script allows the random generation of realistic complex shapes (Figure 1).

We performed a series of single grain crushing simulations, and monitored the force evolution during loading, as well as the remaining cohesive bonds inside the grain in order to determine the exact breakage moment. A characteristic stress was computed using Jaeger's formula [5]. The grain strength depends on the cohesive strength of the bond joining the particles. This result allows us to control the grain's strength for other simulations.

Many samples are then created, in order to simulate œdometric compression tests (Figure 2). A parametric study is carried out, by loading multiple samples with different values of the intra-granular cohesion. A sample of unbreakable grains is also tested. The goal is to evaluate the effect breakage on the macroscopical behavior of the samples, and to study the role of intra-granular cohesion in the breakage process.

Oedometric curves are plotted (Figure 3), grain size distributions. Cohesive bonds breakage is

monitored throughout the loading, and the breakage ratio is computed using Einav's formula [6] (Figure 4), in order to follow grain breakage closely. We showed how an increase in the value of the intra-granular cohesion leads to a shift in breakage process.

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Figures

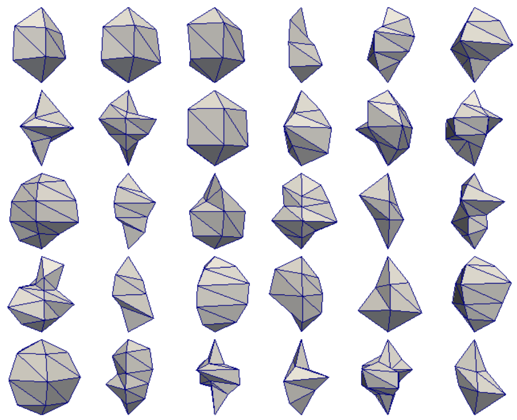

Figure 1. *Randomly generated 3D polyhedral grains*

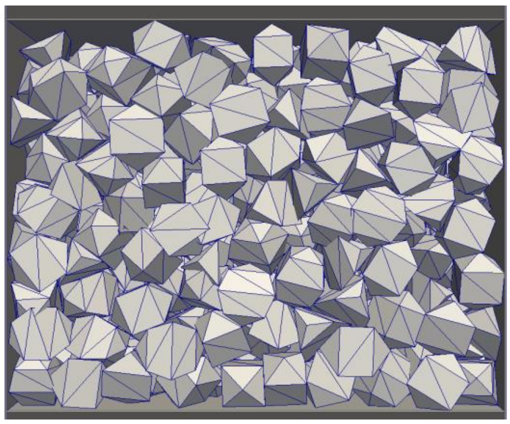

Figure 2*. Sample subjected to oedometric compression*

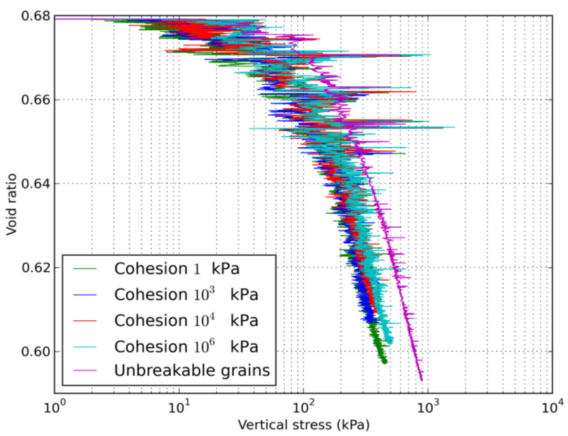

Figure 4*. Breakage ratio as a function of cohesion*

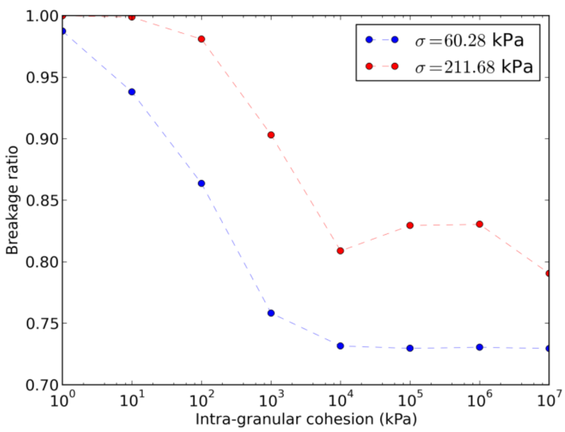

Figure 3*. Oedometric curves for tested samples*

Geomechanical modelling of pore collapsing in soft porous rocks: insights from triaxial experiments and numerical simulations in sandstone, mudstone and shale samples

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Abstract

Understanding compaction and subsidence of reservoirs due to pore-collapsing rocks is vital for the lifetime and performance of the formations. Because of the severe porosity decrease during pore collapse, production rate can be improved due to excess fluid being squeezed out of the formation or vastly impeded due to porosity decrease and/or localized instabilities around the borehole (resulting to sand production etc.). Understanding and modelling the mechanism of pore collapse is therefore key for the performance of a reservoir.

To thoroughly understand pore collapse mechanism we used novel geomechanical approach for modelling pore-collapse using a visco-plastic formulation embedded in a multiphysics framework. A critical mechanical energy threshold (activation energy) required for its activation is attributed to the pore collapse mechanism. This activation energy depends on the pore fluid pressure, ambient temperature and confinement pressure.

In this work we present a novel finite element numerical simulator, REDBACK (Rock mEchanics with Dissipative feedBACKs) that is capable of solving the aforementioned metaphysical approach in a tightly coupled parallel manner experiencing.

We demonstrate the approach by modelling pore collapse and validating the approach against isotropic consolidation experiments on Bleurwiller sandstone as well as drained triaxial experiments on a diatomaceous mudstone and shale rocks for varying confining pressure from heavily over-consolidated to normally consolidated samples and we have captured the common features of all these rocks that have shear bands at low confinement transitioning to compaction bands at high confining pressure.

By modelling the drained triaxial experiments for different rocks, and reproducing the response curves and failure patterns of the samples, we identify the key parameters controlling pore collapse in these rocks. We deduce that the dependency of the pore-collapse's activation threshold on confining pressure is the dominant mechanism reconciling the experimental observations. The results show that dilatancy corresponds to internal processes with negative activation volume, while contractancy corresponds to internal processes with positive activation volume.

This calibration process demonstrates the importance of a physics-based approach in a multi-scale framework, where one can aim at extrapolating results outside the range of laboratory experiments based on the understanding of the underlying physical processes, when traditional engineering approaches are often limited to interpolation within the scope of sparse and expensive experiments.

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