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DEM modelling of highly porous soft rocks

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Abstract: A novel bond damage model is proposed to better replicate the behaviour of highly porous soft-rocks. The contact model employs an exponential damage law to describe the permanent deformation developing at the microscale. To i) reach a high porosity initial state, ii) reproduce complex contact configuration of irregular grains and iii) consider the physical existence of fractured bond fragments, a far-field interaction is introduced in this model, enabling non-overlapping particles to transmit forces. The model performance is validated by replicating the behaviour of Maastricht calcarenite. Finally, a 3D coupled DEM (Discrete Element Method) - FDM (Finite Difference Method) modelling is employed to simulate the penetration of a cone-end shaped pile in calcarenite. The good agreement between the experimental and numerical results suggests that the proposed model has the potential to reveal microscopic mechanism of soft-rock / structure interaction.

1. Introduction

Soft rocks typically exhibit poor mechanical performance due to their porous microstructure, characterized by non-spherical grains bonded to each other [1] [2]. This highly porous microstructure also makes them prone to the formation of compaction bands. Under stress, the bonds break and the structure collapses, leading to irreversible volumetric changes, transforming the rock into a granular material. Soft rocks exhibit varied responses in the post-peak stage when sheared under different confinements. These responses result from the combination of two competing effects: strain softening induced by bond damage and hardening caused by post-failure particle frictional behaviour [3]. The mechanical complexity of soft rocks contributes to the over-conservatism of current pile design [4].

The Discrete Element Method (DEM) is a numerical tool which explicitly represents individual, discrete soil particles. Therefore, it can deal with extreme large deformations and at the same time offer a microscopic view of ground-foundation interaction. Matching the extremely high porosity structure (>50% porosity) of soft rocks in DEM is crucial for properly capturing its collapsible, strain-softening behaviour. When using spherical particles, far-field interaction can be used to capture realistic distribution of physical contacts [9]. Additionally, a physically-based bond damage model is required to reproduce the rock transition from intact to completely remoulded state. Nguyen et al. [10] introduced a bond damage variable related to plastic deformation, and successfully captured the compressive dilation at the contact scale. Building upon this, Senanayake et al. [11] extended this model by adding an extra planar cap, addressing the compressive failure mode. In this context, it is often difficult to capture the ductile failure mechanism exhibited by soft rocks.

In this work, a new contact model able to overcome the difficulties related to modelling cemented highly porous geomaterials with the DEM is proposed. Based on the bond damage model proposed by Zheng et al. [12], the far-field interaction is incorporated to consider the physical presence of bond fragments and complex interaction of irregular particles. After matching the responses of Maastricht calcarenite in element tests, a coupled DEM-FDM approach is employed and the performance of the model to solve Boundary value problems (BVPs) is demonstrated by simulating the installation of a model pile in rock.

2. Far-field interaction

The key to replicating the behaviour of soft rocks in DEM modelling lies in capturing the transition from a rock-like to a granular material-like response. This requires accurately balancing the effects of the bond damage process and the successive frictional interaction between unbonded particles. After bond failure, particle rotation is inhibited in order to overcome the classic lack of particle interlocking issues that plague sphere-based DEM. Two types of contact forces—bonded and unbonded forces—are incorporated into the model. The calculation of bonded forces ($N, V, \breve{M}$) and related equations are listed in equation 1 and 2, where u_n, u_s and θ_b are the deformation of the bond and superscript p indicates the plastic part. Unbonded particles follow the same model, without accounting for plastic deformations or bond damage. The associated flow rule is accepted in this model to calculate the plastic deformation based on the yield function proposed in equation 3. All the other variables in eqs (2) and (3) represent hardening parameters and yield surface size parameters, respectively. For a detailed description, please refer to Zheng et al. [12]. To avoid significant stress loss, i.e. sample collapse, often encountered using bond damage models to simulate porous rocks (see Fig. 1), this model introduces the far-field interaction and its mechanism is illustrated in Fig. 2. Experimental observations by Ciantia et al. [13] show that when the bonding material fractures into several fragments a portion of this material stays in the gaps, transferring compressive loads between particles not in direct contact, see Figure 2a. However, in DEM simulations, particle bonds do not possess any mass or volume. Therefore, the current model proposes far-field contact, as shown in Fig. 2a, to consider the physical presence of some active fragments. Additionally, Figure 2b presents another situation where far-field contact is required, enabling reproducing a more realistic contact distribution between simplified spherical particles [9]. The triggering of these two far-field contact conditions is controlled by the activation gap g_a. To simplify the subsequent model calibration, it is assumed that g_a for both far-field contact conditions is the same and calibrated through matching the initial state of the unbonded sample.

The effect of this far-field contact is evaluated through isotropic simulations on soft rocks. Figure 1 illustrates that samples incorporating far-field interaction are able to capture the ductile failure of porous soft rocks.

$$\begin{bmatrix} N \\ V \\ \breve{M} \end{bmatrix} = \begin{bmatrix} k_n(u_n - u_n^p)A \\ k_s(u_s - u_s^p)A \\ k_b(\theta_b - \theta_b^p)/\bar{R} \end{bmatrix} = \begin{bmatrix} (1-D)k_n^0(u_n - u_n^p)A \\ (1-D)k_s^0(u_s - u_s^p)A \\ (1-D)k_b^0(\theta_b - \theta_b^p)/\bar{R} \end{bmatrix} \tag{1}$$

$$D = 1 - e^{-\left(\frac{|u_n^p|}{u_n^c} + \frac{u_s^p}{u_s^c} + \frac{\theta_b^p}{\theta_b^c}\right)} \tag{2}$$

$$f = \left(\frac{\breve{M}}{\overline{\overline{\widetilde{M}}}}\right)^{1.001} + \left(\frac{N}{\overline{\overline{N}}}\right)^2 + \left(\frac{V}{\overline{\overline{V}}}\right)^4 \left[1 - \left(\frac{N}{\overline{\overline{N}}}\right)^2\right]^{-1} - 1 \tag{3}$$

3. Model performance

In this study, a typical porous soft rock — Maastricht calcarenite — is used to calibrate the proposed model. Utilizing the particle size distribution (PSD) provided by Zheng et al. [12], a cylindrical sample with a porosity of 0.52 is generated. The dimension of the numerical sample is 1.2*2.4mm. The final calibrated values are summarized as follows: the effective modulus for bonded and unbonded contacts is $\bar{E}_{mod}$ =2.5 GPa and E_{mod} =0.63 GPa, respectively; the normal to shear stiffness ratio is 2.4. The compressive strength, tensile strength, and cohesion are 22 MPa, 4.0 MPa, and 4.5 MPa, respectively. The softening parameters for normal (shear) and rotational loading are 0.061d_{00} and 0.04. The final activation gap g_a is 0.13 d_{00}. Corresponding calibrated results are presented in Figure 3, demonstrating the model's capability to capture void collapse and its ability to predict the experimentally observed transition from softening to hardening when shearing the rock under both low and high confinements.

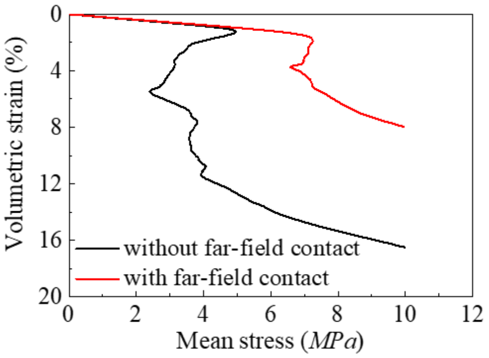

Figure 1. Effect of far-field interactions.

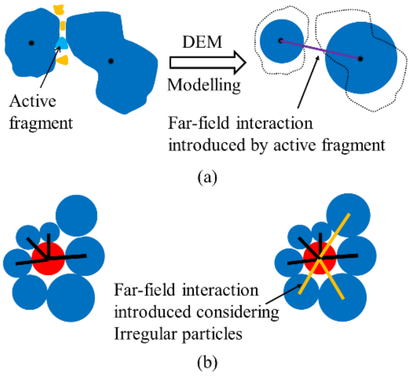

Figure 2. Schematic diagram of the far-field interactions introduced by (a) active bond fragments and (b) considering irregular grains.

A cylindrical coupled DEM-FDM model is generated to simulate the penetration of a cone-ended pile penetrating into the rock. The dimensions of the coupled model are illustrated in Figure 4 (pile diameter of 1mm). An elastic constitutive model is adopted for the FDM region due to the small-deformation response in the far field. The contacts between the pile and particles are modelled as unbonded linear contacts, with a friction coefficient of 0.2 between the pile and calcarenite (Ziogos et al., 2023). As shown in Fig 4 the model captures very well the experimental data [14] in terms of load displacement, showcasing a promising potential for simulating Boundary Value Problems in porous soft rocks.

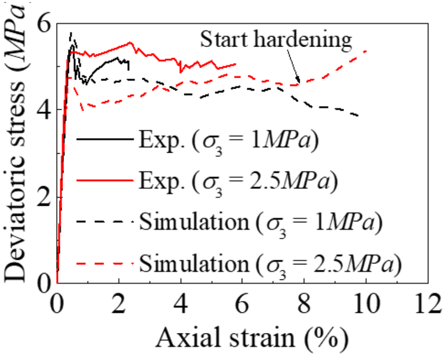

Figure 3. Calibrated result.

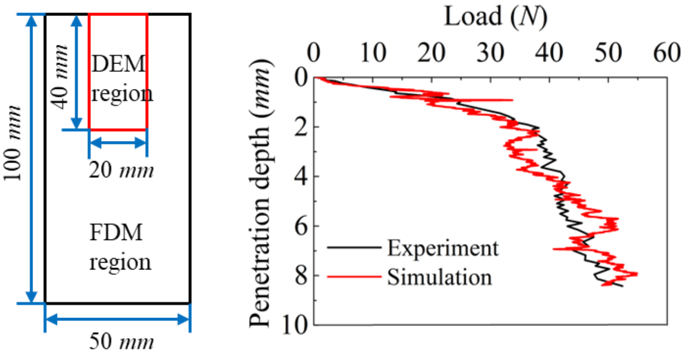

Figure 4. Model size and load-displacement curve.

4. Conclusions

In this paper a novel DEM contact model for highly porous rocks, with a focus on capturing yielding and post-yield behaviour under various confinements (while providing micromechanical insights into rock-structure interactions), is proposed. The model introduces a far-field interaction concept allowing simulation of highly porous rocks whilst using spherical particles. Based on the appropriate bond damage criterion, a transition from an intact (rock-like) to a completely broken (granular-like) state is observed through calibration against Maastricht calcarenite. Finally, it's performance is validated at the model test scale by simulating pile penetration in the same soft rock.

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