A coupled damage-plasticity DEM bond contact model for highly porous rocks

Zheng, Jinhui; Ciantia, Matteo; Previtali, Marco; Knappett, Jonathan

Published in:
Proceedings of the 2024 UK Association for Computational Mechanics Conference

Publication date:
2024

Document Version
Publisher's PDF, also known as Version of record

A coupled damage-plasticity DEM bond contact model for highly porous rocks

Jinhui Zheng*, Matteo Ciantia, Marco Previtali, Jonathan Knappett

School of Science and Engineering, University of Dundee, Dundee, DD1 4HN, UK.
2431370@dundee.ac.uk

Abstract

In view of the significant stress loss induced by stuructural collapse when simulating high-porous soft rocks using traditional damage bond models in DEM (discrete element methd) modelling, a novel damage bond contact model is proposed to capture the ductile failure of high-porous cemented soft rocks. To address the unrealistic physical contact distribution resulting from the use of spherical particles in DEM modelling and consider the physical presence of broken bonds, far-field interaction is introduced between grains when two untouched particles reach a specific activation gap, enabling the genration of stable, highly porous open structure samples while using spherical DEM particles. The final results demonstrate that this newly developed model facilitates the transition from the purely elastic rock-like behaviour stage to the transitional ductile failure stage of porous soft rocks, as well as reproduces the softening/hardening response of soft rocks under different confinements.

Key words: *DEM contact model; High-porous bonded soft rock; Far-field interaction; Micro mechanics.*

1 Introduction

In general, rocks with an unconfined compressive strength (UCS) within the range of 0.5 to 25 MPa are collectively referred as soft rocks [1]. Typical examples include chalk, calcarenites and porous tuffs. Typical microstructure of soft rocks is usually characterised by angular grains connected by a chemical bond formed during their sedimentation and diagenesis process. This configuration often leads to a high-porous structures characterized by inter and intra-granular voids. Due to this, soft rocks exhibit unique mechanical responses, showing elastic rock-like behaviour transitioning to soil-like behaviour induced by the damaged microstructure during loading [2]. Under triaxial loading conditions, the behaviour depends on the confinement, as two competing effects develop in the sample: i) softening induced by bond degradation and ii) hardening attributed to the granular structure resulting from the rearrangement of particles. These two microscale effects are at the base of the complex behaviour oof soft rocks.

In recent years, there has been a growing trend in constructing engineering projects on porous rocks. For example, monopiles supporting offshore wind turbines built on the chalk in the North Sea [3] require a more economic foundation design while the intricate mechanical characteristics of high-the material poses challenges in assessing foundation bearing capacity, often leading to conservative designs. From a numerical perspective, the key to developing an improved foundation design lies in using advanced models enabling a comprehensive reproduction the complicated mechanical behaviour. Over the past few decades, several constitutive models based on plasticity theory and considering damage to cemented bonds, as well as models considering bond degradation based on macro-element method, have been proposed [4] [5]. However, these models regard soft rocks as continuous mediums and would require continuum modelling frameworks able to manage discontinuities and large deformations. These include PFEM [6], MPM [7], XFEM [8].

As an effective approach to address discontinuity issues, there are currently numerous models developed based on the DEM to describe the behaviour of cemented soft rocks. These models primarily focus on replicating the damage induced softening of cemented bonds to capture the ductile failure of soft rocks. For example, Nguyen et al. [9] proposed a damage bonded model by considering the bond damage caused by tension and shearing, where the evolution of bond damage follows an exponential damage law attributed to the plastic deformation of the bond. Subsequently, a new model incorporating compressive damage was developed by Senanayake et al. [10] based on Nguyen et al. [9]'s work. Zheng et al. [11] provided a damage DEM model for bonded rocks that can reflect bond damage caused by compression, tension, shearing and rotation. Nonetheless the above-mentioned models are still limited in comprehensively capturing the behaviour of high-porous soft rock because unbonded contacts are only created after bonds breakage, resulting in significant stress loss in numerical samples during loading. In reality, bond degradation is a progressive process, and the initial intact bond can be degraded into several segments [12], some fragments can still transfer the load even though the bond structure is completely broken. To improve the computational efficiency, most DEM models do not incorporate bond fragments in the model, leading to the inability of numerical broken bonds to transfer the load. In addition, most DEM models use spherical particles to decrease computational burden, hence posing significant challenges in capturing realist porosities of the remoulded rock.

To comprehensively consider the physical presence of broken bonds and contact distribution of irregular particles, a far-field interaction is introduced based on Zheng et al. [11]'s damage model. The performance of this newly developed model is then evaluated through simulating isotropic and triaxial tests, showcasing its promising ability to capture the typical behaviour of high-porous bonded soft rocks.

2 Limit of current damage bond model

Although current damage model has been proven to reproduce the response of soft rocks in both lab and BVP (boundary value problem) tests, its ability to reproduce the behaviour of high-porous soft rocks (porosity >0.5) still needs to be investigated. Triaxial ($\sigma_3 = 1\text{MPa}$) and isotropic tests are simulated to demonstrate the incapability of current damage models to simulate high-porous rocks (porosity=0.52). The PSD of the numerical sample can be found in Zheng et al. [11]. A cylinder-shaped numerical sample is created, comprising approximately 18k particles, with dimensions of 240mm in height and 120mm in diameter with an upscaling ratio is 50. Where interparticle bonded contact forces are calculated based on Zheng et al. [11]'s work and related model parameters are summarized in Table 1. As indicated in the table model parameters listed can be categorized into three families. *Elastic parameters*, which includes the particle effective modulus (bond effective modulus) E_{mod} ($\bar{E}_{mod}$) and the particle normal-to-shear stiffness (bond normal-to-shear stiffness) κ^*($\bar{\kappa}^*$). *Strength parameters*, including tensile strength σ_t, compressive strength σ_t and cohesion C. *Softening parameters* u_c^n, u_c^s and θ_c^b, controlling the bond damage rate in the normal, shear and rotation directions.

Simulated results are shown in Fig. 1. Unlike the ductile failure observed in most experiments (see Fig. 1 left from Lagioia & Nova [2]), a completely stress loss happens after initial elastic stage in both two elements tests (Fig. 1 middle and right). In isotropic tests, samples need to undergo significant compression deformation to restore the previous stress level. From a microscopic perspective, this is because, during the fracture of most bonds, the physical contacts between particles are not sufficient, and numerical samples cannot establish a stable microscopic structure to withstand external loads. Slowing down the softening rate of bonds slightly decreases the effect, but not sufficiently to properly reproduce the post-peak observed. Moreover decreasing the softening rates lead to non-realistic shearing responses.

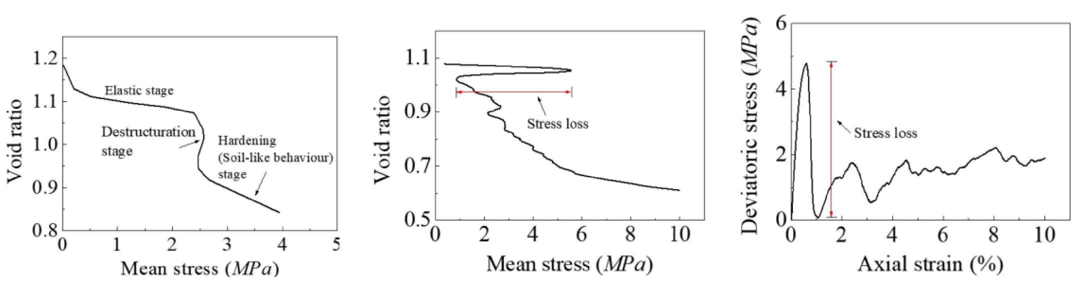

Fig. 1: Experimental (left) and simulated (middle and right) isotropic and triaxial tests without far-field interaction.

3 Far-field interaction

To replicate the behaviour of high-porous soft rocks in DEM modelling is important to capture the rock response during the destructuration stage. Capturing the collapse caused by bond breakage and accurately account for the introduction of unbonded contacts is key. To overcome the limitations shown in the previous section the concept of far-field interaction is introduced.

An irregular intact bond fractures into several fragments, with some active fragments capable of transferring load between grains even after bond breakage. However, in DEM modelling, broken bonds are deleted. To replicate this process, far-field interaction is here introduced to consider the physical existence of broken active fragments, as shown in Fig. 2. The introduction of far-field interaction replaces the function of transiting interparticle loads by active segments of the fractured bond, without affecting the computational efficiency of the model. Furthermore, Fig. 2 also presents another scenario to account for the far-field interaction—physical contact due to irregular particles in real rock samples. The use of spherical particles cannot accurately replicate a genuine physical contact distribution, as there should be more physical contacts surrounding a specific grain compared to when using spherical particles. A similar concept has been reported in Hentz et al. [13]. The unboned contact force introduced by the far-field interaction is updated incrementally according to the linear contact model, while the bonded contact is calculated following Zheng et al. [11]'s model, the total contact force of the contact is the sum of these two types of contact forces.

Table 1. Model related parameters.

Parameter	Family	Value
$\boldsymbol{E_{mod}}$	Elastic	$0.83GPa$
$\boldsymbol{\overline{E}_{mod}}$		$4.5GPa$
$\boldsymbol{\kappa^*(\overline{\kappa}^*)}$		4.5
$\boldsymbol{\sigma_c}$	Strength	$30MPa$
$\boldsymbol{\sigma_t}$		$10\ MPa$
$\boldsymbol{C}$		$10\ MPa$
$\boldsymbol{u_c^n\ (u_c^s)}$	Softening	$0.0305d_{00}\ m$
$\boldsymbol{\theta_c^b}$		$0.01rad$

Far-field interaction in DEM modelling entails generating unbonded contacts between untouched spherical particles. The activation timing of the far-field interaction depends on the gap between two particles, denoted as g_a. To investigate the effect of far-field interaction, setting $g_a = 0.17d_{00}$ based on the numerical bonded sample created in section 2, where d_{00} is the minimum particle diameter of the rock grains. The results, with and without the far-field interaction, are compared in Fig. 3. In contrast to the results in Fig. 1, introducing the far-field interaction leads smaller stress loss allowing to achieve a transition from brittle to ductile failure of the sample. Furthermore, the numerical sample replicates similar responses to high-porous soft rocks under different confinements. As for typical experiments in the literature (data in Fig.3 right from Lagioia & Nova [2]), the sample subjected to 4 MPa confinement exhibits a typical three-stage response (elastic-destructuration-hardening), while the sample under 1 MPa confinement shows a continuous softening.

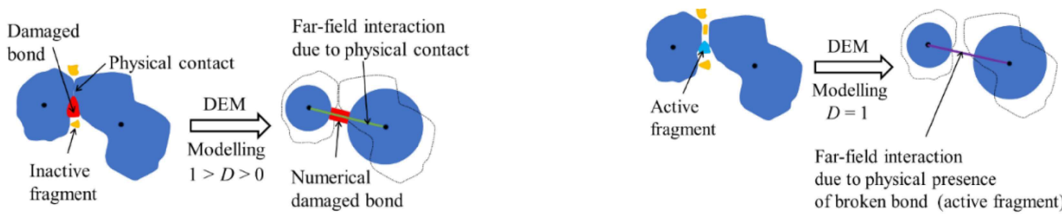

Fig. 2: Schematic diagram of the far-field interaction: (left) Far-field interaction considering the physical contact of irregular particle and (right) considering the physical presence of broken bond.

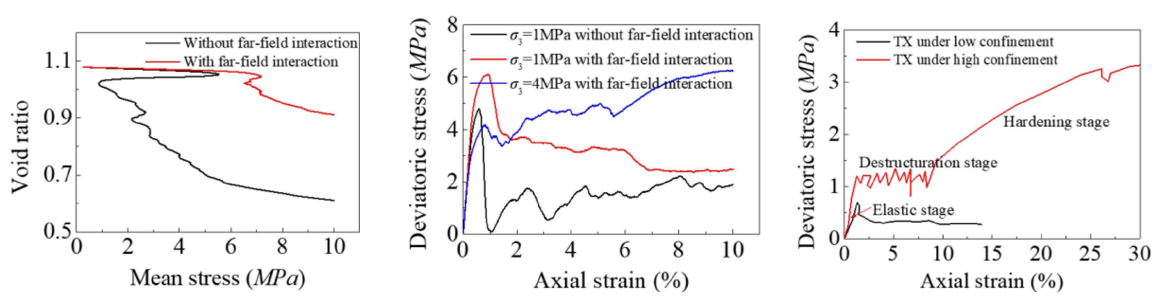

Fig. 3: Simulated isotropic (left) and triaxial (middle) tests without far-field interaction; typical experimental TX response (right).

4 Conclusions

To address the brittle failure when simulation high-porous soft rocks using DEM, the concept of far-field interaction is introduced to account for the physical presence of bonds fragments. Such far-field interaction enables the rock's response to transition from rock-like to soil-like without stress loss whilst still using spherical particles. The model is shown to be able to capture diverse shearing responses of soft rocks under varying confinements. This highlights the potential of the newly developed damage bond model to accurately replicate the behaviour of high-porous soft rocks for large scale simulations.

Acknowledgments

This work is an output from the ICE-PICK project, funded by the New Investigator Award EPSRC grant EP/W00013X/1. Also thanks to the CSC scholarship (202008330363) to support the first author's study.

References

[1] Johnston, I. W. (1991). Geomechanics and the emergence of soft rock technology. *Australian Geomechanics*, 21, 3–26.
[2] Lagioia, R., & Nova, R. (1995). An experimental and theoretical study of the behaviour of a calcarenite in triaxial compression . *Geotechnique*, 45(4), 633–648.
[3] Buckley, R. M., Jardine, R. J., Kontoe, S., et al. (2018). Effective stress regime around a Jacked steel pile during installation ageing and load testing in chalk. *Canadian Geotechnical Journal*, 55(11), 1577–1591.
[4] Ciantia, M. O., & Di Prisco, C. (2016). Extension of plasticity theory to debonding, grain dissolution, and chemical damage of calcarenites. *International Journal for Numerical and Analytical Methods in Geomechanics*, 40(3), 315–343.
[5] Nova, R., & Parma, M. (2011). Effects of bond crushing on the settlements of shallow foundations on soft rocks. *Geotechnique*, 61(3), 247–261.
[6] Carbonell, J. M., Monforte, L., Ciantia, M. O., et al. (2022). Geotechnical particle finite element method for modeling of soil-structure interaction under large deformation conditions. *Journal of Rock Mechanics and Geotechnical Engineering*, 14(3), 967–983.
[7] Coombs, W. M., Augarde, C. E., Brennan, A. J., et al. (2020). On Lagrangian mechanics and the implicit material point method for large deformation elasto-plasticity. *Computer Methods in Applied Mechanics and Engineering*, 358, 112622.
[8] Belytschko, T., & Gracie, R. (2007). On XFEM applications to dislocations and interfaces. *International Journal of Plasticity*, 23(10–11), 1721–1738.
[9] Nguyen, N. H. T., Bui, H. H., Nguyen, G. D., et al.. (2017). A cohesive damage-plasticity model for DEM and its application for numerical investigation of soft rock fracture properties. *International Journal of Plasticity*, 98, 175–196.
[10] Senanayake, S. M. C. U., Haque, A., & Bui, H. H. (2022). An experiment-based cohesive-frictional constitutive model for cemented materials. *Computers and Geotechnics*, 149, 104862.
[11] Zheng, J., Previtali, M., Ciantia, M.O., et al. (2023). Micromechanical Numerical Modelling of Foundation Punching in Highly Porous Cemented Geomaterials in a Virtual Centrifuge Environment. In Palermo (Ed.), *CNRIG 2023* (pp. 390–397).
[12] Ciantia, M. O., Castellanza, R., Crosta, G. B., et al. (2015). Effects of mineral suspension and dissolution on strength and compressibility of soft carbonate rocks. *Engineering Geology*, 184, 1–18.
[13] Hentz, S., Donzé, F. V., & Daudeville, L. (2004). Discrete element modelling of concrete submitted to dynamic loading at high strain rates. *Computers & Structures*, 82(29), 2509–2524.