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Discrete particle methods for granular bentonite material simulation

Joel Torres-Serra[1,2,*], Enrique Romero[2] and Vicente Navarro[1]

[1] Geoenvironmental Engineering Group, Universidad de Castilla-La Mancha, Ciudad Real, Spain
[2] Department of Civil and Environmental Engineering, Universitat Politècnica de Catalunya, Barcelona, Spain
* Corresponding author: joel.torres@uclm.es/joel.torres@upc.edu

Bentonite clays are strategic materials to ensure the sealing capacity of engineered barrier systems (EBS) in deep geological repositories of high-level radioactive waste. Formerly installed in the form of compacted blocks, in recent years, there has been growing interest in EBS design using granular bentonite materials (GBM) due to improved construction processes [1]. GBM range from the powdered and granulated forms, both natural and obtained from crushed blocks, to compressed bentonite pellets, and the mixtures thereof. The effect of thermo-hydro-chemo-mechanical (THCM) conditions on the evolving gap-filling performance following installation has been investigated in full-scale experiments [2] and in laboratory-scale tests [3], with particular focus on bentonite pellet-powder mixtures [4, 5, 6].

Numerical modelling of coupled THCM expansive soil behaviour is widespread using continuum methods, namely the finite element method [7, 8], applicable up to full-scale systems even though at the expense of resolution. At the laboratory scale, discrete particle-based methods accounting for the granular nature of bentonite materials in the early stages of hydration provide insight into pellet shape and local effects on the mechanical behaviour of dry pellet-powder systems as well as hydro-mechanical effects on the swelling capacity of GBM systems.

The compressibility of dry pellet packings and pellet-powder mixture samples is modelled by the discrete element method (DEM). This method has been applied to study the swelling behaviour of pellets represented by spherical particles [9]. The DEM is a powerful tool for reproducing complex granular shapes by non-spherical particle surfaces [10] and also with clumps of spheres (Figure 1(a)), allowing to define mixed material and mechanical contact properties within the pellets. The deformation and fissuring of pellets under oedometer compression is tracked using a cohesive particle model [11], including damage for interparticle contacts in tension, which captures deformation associated phenomena such as surface spalling and pellet reorganisation occurring at stress levels below the diametral fracture. In addition, bentonite powder is represented by loose packings of upscaled spheres matching

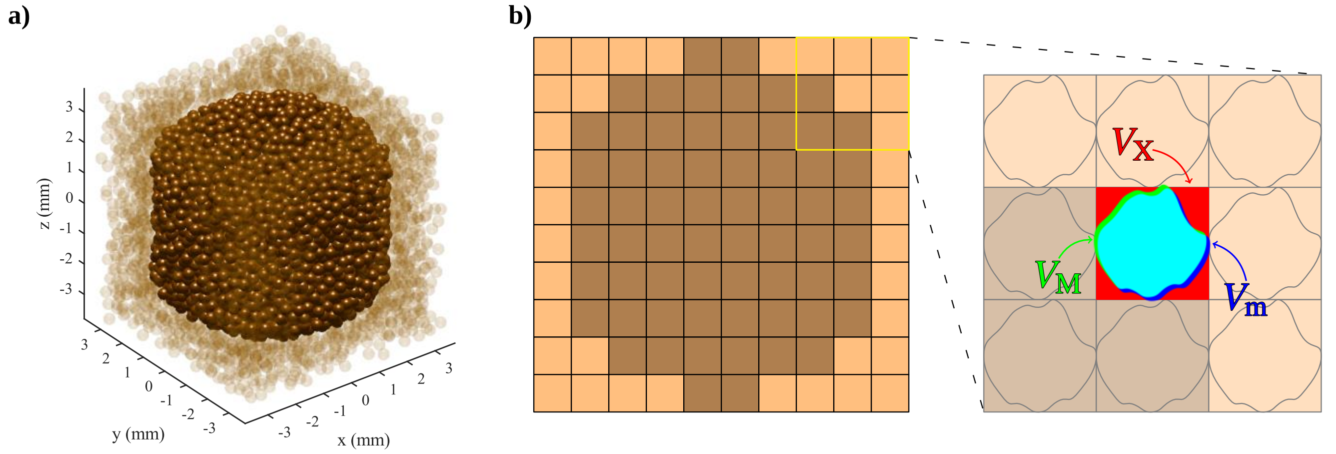

Figure 1: Discretisation of bentonite pellet-powder systems: a) spherical particles by the DEM; b) bentonite units by the XMm method.

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the experimental porosity of the fillings, interacting by a classical linear spring-dashpot contact model resulting in the reduced overall compressibility observed in pellet-powder mixtures [5].

Flow through GBM systems is modelled by the new discrete particle-based XMm method [12]. In the XMm, the material is discretised into a set of bentonite units (BU) or particles acting as representative elementary volumes of a homogeneous continuum inside which the mass balance equations are solved at the megastructural (X), macrostructural (M), and microstructural (m) pore levels (Figure 1(b)). Moreover, the mechanical compatibility of the system is obtained from the coupling between strain increments and centroid displacements in each BU, where the contact stress and overlap between neighbouring particles are updated similarly to the DEM approach. The hydro-mechanical problem is posed as a set of ordinary differential equations (ODE) to be solved for each BU, and thus the efficiency of the XMm is a compromise between the typically reduced computational cost of ODE solvers and the number of BU considered. The XMm has been used to simulate the hydration of a powder sample with low heterogeneity [4], successfully capturing the evolution of the displacement field upon saturation in isochoric conditions. This method is applied to reproduce the confined hydration of a heterogeneous pellet-powder system [6]. Assuming 2D axisymmetry, the XMm allows defining different initial material properties in each BU introducing the heterogeneity of the sample. The evolving swelling pressure is reproduced as well as the hydration velocities at the different structural levels, showing the decreasing heterogeneity of the mixture.

Contributor statement

Conceptualisation: Joel Torres-Serra (JTS), Enrique Romero (ER), Vicente Navarro (VN); funding acquisition: JTS, ER, VN; investigation: JTS, ER, VN; methodology: JTS, ER, VN; resources: ER, VN; software: JTS, VN; supervision: ER, VN; validation: JTS, ER, VN; visualization: JTS; writing – original draft: JTS; writing – review & editing: ER, VN.

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