Understanding particle-scale mechanisms in clays: a virtual experimental investigation using DEM

Micro-scale processes occurring in clayey geomaterials cannot be easily investigated in a direct fashion due to the small size of clay particles, as opposed to granular materials. This poses a severe limitation to the understanding of the particle-scale phenomena responsible for the overall macroscopic response of clays. A suitable approach to overcome this issue and to gain insight into clay micro-mechanical behaviour would consist of performing 'virtual' experiments within a Discrete Element Method (DEM) framework.

This work presents a few applications of a simple, two-dimensional DEM framework designed on the basis of 'indirect' experimental evidence at the microscale (Scanning Electron Microscope, Mercury Intrusion Porosimetry), rather than the theoretical formulations of interparticle interactions. The piece-wise linear contact laws implemented in the adopted DEM framework account for both the mechanical interaction developing between particles in contact, and the long-range electro-chemical interaction in the form of Coulombian attraction/repulsion between charged particles not yet in contact.

The DEM framework is proved to reproduce qualitatively some key aspects of the macroscopic behaviour of non-active clays observed experimentally in various conditions. First, the effect of different pH and dielectric permittivity of the pore-fluid on the initial void ratio of unloaded specimens, resulting from changes in the interparticle interactions, is successfully captured. Then, the macroscopic responses of the same specimens during one-dimensional compression, simple shearing and elastic shear-wave propagation observed experimentally are successfully reproduced by the virtual specimens. It is shown that the analysis of the simulation data at the micro and meso-scale (particle arrangements and orientations, fabric, force chains etc.) may be used as a valuable tool to investigate particle kinematics and force transmission mechanisms, and to link specific particle-scale processes to their effect(s) at the macroscopic scale.