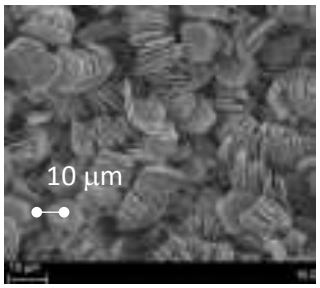
Fundamental analysis of the influence of structure on clay behaviour

PhD Studentship

Imperial College London

Start date: Oct 2017



Scanning electron microscope image of kaoliniate clay

Clay is a type of soil with fine grains that have specific chemical compositions (mineralogies). It constitutes an estimated 16% of the volume of material at the surface of the earth. The behaviour of clay is complex and its presence, even in small concentrations, can strongly influence the mechanical properties of a soil. Geological processes determine many aspects of a clay's structure, such as the relative orientations and arrangements of clay particles, and the nature of any chemical bonding between them. We would like to better understand how a clay's structure determines its behaviour. In particular, we would like to use a novel particle-scale modelling approach to explain macro-scale observations reported in recent seminal research.

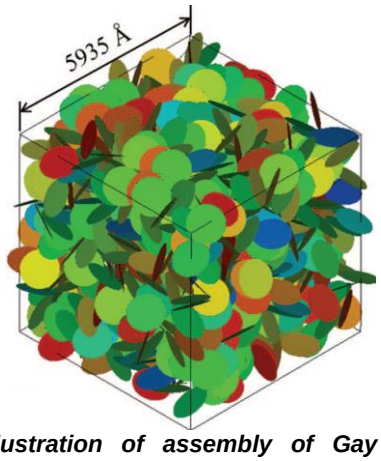


Illustration of assembly of Gay Berne ellipsoids to represent clay by Ebrahimi et al. (2014)

Much can be understood about a clay's microscopic structure from scanning electron microscopy (see image above). The sensitivity of the macro-scale behaviour of clay to its microscopic structure has become clear by comparing the mechanical properties of clays with different microscopic structures. Although some useful phenomenological explanations of how structure relates to macro-scale properties have been proposed, they are difficult to fully validate. They also lack detail and so they provide limited fundamental insight. A very promising route to a deeper understanding is to develop an accurate microscopic model of clay particles, their orientations, and their interactions, and then to use this model to calculate or to simulate macroscopic properties. If good agreement with both microscopic and macroscopic experimental observations can be achieved from this bottom-up approach, one can have much more confidence in its validity. Furthermore, it would provide a more detailed and fundamental understanding – perhaps even enabling macroscopic properties to be engineered by tuning microscopic structure. This approach has been used to improve our understanding of sand behaviour. However, because sand grains are relatively large (heavy), the weak interactions between surfaces of grains can be neglected. By contrast, the larger surface-to-volume ratios of clay particles means that surface 'stickiness' can measurably influence a clay's behaviour.
The proposed research will apply molecular dynamics, which is a modelling technique used in physics, chemistry and materials science, to study structure effects on clay. Some recent progress has been made in this area, e.g. Ebrahimi et al. (2014), which demonstrates the project viability. The specific aim of this research is to capture the sensitivity to structure observed in laboratory tests and to use the results to examine previously-proposed continuum models of structure effects.

Funding has been provided for a 42 month PhD studentship for UK / EU students by the Leverhulme Trust. The PhD student will be co-supervised by Dr. Catherine O'Sullivan (Civil Engineering), Dr. Paul Tangney (Materials / Physics) and Dr. Stefano Angioletti-Uberti (Materials). An external group of

experts will review the project and provide additional guidance and technical support. Suitable applicants will have undergraduate degree in either materials, civil engineering or physics. For further details email Catherine O'Sullivan: cath.osullivan@imperial.ac.uk

Reference

Ebrahimi, D., Whittle, A.J. & Pellenq, R.J.-M., 2014. Mesoscale properties of clay aggregates from potential of mean force representation of interactions between nanoplatelets. The Journal of Chemical Physics, 140, p.154309. Available at: http://dx.doi.org/10.1063/1.4870932.