Ph.D.: Mechanics of swelling clay faults from molecular simulation to earthquakes

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Context

Plate boundary fault zones exhibit a wide range of dynamic behaviors, from aseismic slip to mega-earthquakes. So far, there is no consensus on a model describing the processes controlling these fault behaviors. A possible answer might lie in the properties of smectite, a swelling clay mineral that form the core of many of the fault zones and that is able to adsorb significant amounts of water in-between nanometric minerals. Despite their potential importance, the thermodynamics of hydration/dehydration reactions in smectite and the connections between these reactions and the fault deformations, is not yet known. These fundamental questions are the heart of the ANR project SMEC funding this Ph.D. position.

The objectives of the SMEC project are: 1) to decipher the thermodynamics of hydration/dehydration in smectite, as a function of the conditions of confining pressure, fluid pressure, and temperature, 2) to link hydration to the mechanical behavior, and 3) to upscale this coupling between hydration and mechanics to the scale of faults in the perspective of applying it to address large-scale natural examples. These questions will be addressed using a combination of laboratory experiments and numerical simulations from the clay mineral layer to the fault.

Objective

This Ph.D. project focuses on the modeling of part of the SMEC project. More precisely, we propose to combine molecular simulations, granular modeling and micromechanics in order to relate the hydration/dehydration reactions of smectites to the mechanical behavior of faults zones. Recent advances in molecular modeling provide realistic atomistic models of clay, that are able to capture reasonably well the swelling behavior at the nanometer scale under arbitrary confining stress, water pressures and temperatures[1]. Yet, the interplay between hydration and mechanics, in particular regarding the response to shearing, is poorly known, and will be the first objective of the Ph.D. project. Particular attention will be paid to investigate the hydration states representative of fault conditions, and the corresponding results will be confronted to lab and synchrotron XRD measurements under in-situ conditions that are planned in the SMEC projects (not handled in the present Ph.D.).

The second objective of the Ph.D. will be the up-scaling from the nanometer to the fault material. In this respect, the Ph.D. project will build on a recent granular model of clays[2], coarse-grained from the molecular scale, that is able to capture both hydration and mechanics at the scale of the clay matrix (< µm). While the mechanics at the nanoscale has little to do with the macroscopic behavior, the mechanics

[1] Brochard, L. (2021) Swelling of Montmorillonite from Molecular Simulations: Hydration Diagram and Confined Water Properties. Journal of Physical Chemistry C 128, 15527-15543.

[2] Asadi, F., Zhu, H.-X., Vandamme, M., Roux, J.-N., & Brochard, L. (2022). A meso-scale model of clay matrix: the role of hydration transitions in geomechanical behavior. Soft Matter, 18(41), 7931-7948.

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at the matrix scale already exhibits most features of usual clay mechanics (plasticity, logarithmic response to compression, thermal compaction). Yet, this granular modeling is limited to pure clays, while fault zones are mixture of swelling and non-swelling clay, and also contain other non-clay minerals. In this respect, the granular modeling will be complemented by micromechanics to evaluate the effect of mineral composition. Again, the up-scaling results will be confronted to triaxial experiments planned in the SMEC project (not handled in the present Ph.D.).

Practical information and applications

This Ph.D. project will be located at Navier laboratory (Champs-sur-Marne, Paris region), with occasional travels (SMEC project meetings, conferences). The Ph.D. candidate will be enrolled in the doctoral school 'Science, Ingénierie, Environnement' of the Ecole des Ponts ParisTech, and will be funded by CNRS within the scope of the ANR SMEC. The Ph.D. funding is granted for a total of three years with a gross stipend of 2135€/month for full time work. The start of the Ph.D. is flexible but it cannot be before 1st January 2024.

The applicants must hold a Master of Science or equivalent in the field of physics and/or (geo)-mechanics of materials (or close subject), with a special taste for numerical work. They must be able to communicate fluently in English, both written and spoken. The interested applicants are invited to apply on the CNRS career portal (https://emploi.cnrs.fr/Offres/Doctorant/UMR8205-LAUBRO-002/Default.aspx?lang=EN) or by email by sending a CV, a motivation letter and their transcripts to L. Brochard (laurent.brochard@enpc.fr).

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