PhD project

THM modeling of claystone from the molecular scale

L. Brochard, A. Pouya –Navier Lab., Ecole des Ponts ParisTech

Context

Claystone is a highly heterogeneous material and their finest mineral (clay) is made of nanometric particles for which the molecular interactions between interstitial water and minerals are essential to the understanding of the poro-mechanical behavior. The pressure of this bound water (adsorbed) differ very significantly from the usual pressure, the difference is generally referred to as the disjoining pressure. The disjoining pressure is at the origin of various unusual mechanical behaviors of clays, in particular the phenomena of drying shrinkage, of thermal compaction (normally consolidated clays), or of excess water thermal pressurization. The macroscopic consequences are numerous, the most well-known being the desiccation cracking. In the context of CIGEO (nuclear waste geological storage in France), various issues are directly related to the THM behavior of claystone: cracking around galleries, re-saturation around waste packages, pressurization / compaction under thermal loading etc.. The fine understanding of the THM behavior of claystone is therefore an important challenge for the validation of the observations and macroscopic models, and, in fine, for the design and safety of the storage.

However, evaluating the properties of bound water is extremely difficult from an experimental point of view and limited to very well controlled minerals. For about a decade, molecular simulation has become an interesting alternative to experiment, able to provide realistic estimates of the properties at the nanometric scale. However, the time and length scales accessible are highly constrained (tens of nm / tens of ns), so the molecular simulation approach has to be completed by an upscaling approach to be applicable to claystone. In the framework of the ANR project TEAM2ClayDesicc (2015-2019), a first step in that direction was undertaken to relate the bound water to the thermal behavior of saturated clays. The approach considered uses molecular simulation to estimates the thermo-mechanical moduli of bound water, and then a poro-mechanical formulation extended to bound water provides an upscaling which can be confronted to experiment.

The goal of this PhD project is to set up a THM macroscopic modeling of Callovo-Oxfordian claystone that takes into account explicitly the unusual properties of bound water, obtained by molecular simulations of representative clays. The project is organized in three parts: 1- molecular simulation, 2- poromechanical formulation, and 3- confrontation to the state of the art (modeling and experiment)

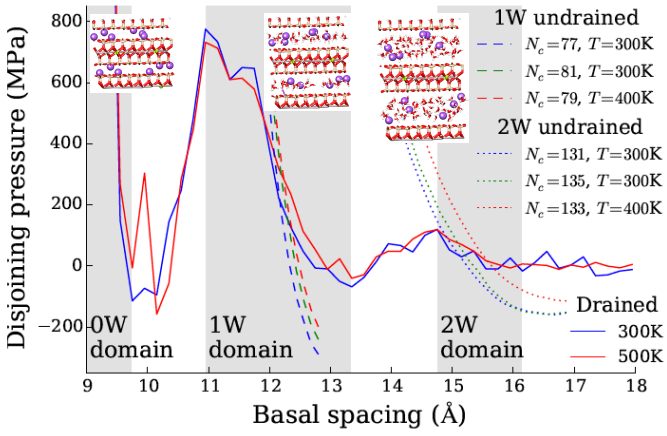

Figure: Disjoining pressure of water in Na-Montmorillonite obtained by molecular simulation[1]

Molecular simulation

We propose to use molecular simulation to establish a database of the properties of bound water in clay minerals representative of the Callovo-Oxfordian claystone. Previous studies (in particular ANR TEAM2ClayDesicc) have provided first estimates and have shown in particular that bound water can be fully described only by taking into account 6 moduli instead of 3 for usual fluids (compressibility, thermal expansion, heat capacity) because the high confinement breaks the extensivity of the fluid (otherwise said, the Gibbs-Duhem equation no more holds for bound water). However, these first estimates were obtained for a

[1] Honorio et al. (2017) Langmuir, 33(44), 12766–12776. http://doi.org/10.1021/acs.langmuir.7b03198

model montmorillonite above the bulk water saturation pressure. We propose to consider the case of minerals representative of COx in conditions corresponding to geological storage.

Poro-mechanical formulation

Taking into account adsorption in poro-mechanics is an active topic of research, which is not limited to claystone[2]. Recent advances make it possible to take into account quantitatively the effect of bound water and its 6 moduli[3]. The practical implementation of the extended poromechanics is rather simple because the structure of the constitutive equations remains the same as in usual poro-mechanics and thus is easily integrated to existing codes. However, if the molecular simulation provides the properties of bound water, one has to determine the properties of the solid skeleton. We propose to calibrate those properties from the inverse analysis of usual tests (e.g., drained compressibility). In this respect, various experimental results on COx (from the literature or from ANDRA) will be considered.

We propose to set up a numerical implementation of this poro-mechanical model base on Discroc[4]. Disroc is a finite element code dedicated in particular to the simulation of fractured porous media. It is particularly adapted to the study of cracking under the effect of complex THM couplings: natural fracturing of sedimentary formations and oil/gas reservoirs[5], desiccation cracking of soils[6], crack propagation under the effect of fluid injection[7]. The implementation in Disroc offers the perspective to simulate various issues of interest with respect to the CIGEO project, and thus to confront the new modeling to existing models and experimental results.

Confrontation with the state of the art

In agreement with ANDRA, the model developed will be confronted to the state of the art in order to assess the influence of addressing bound water explicitly, in contrast with existing approaches. The situations studied will relate in priority on issues for which bound water is known to be at the heart of the THM couplings.

Practical details and applications

The applicants must hold a Master of Science or equivalent in the field of mechanics and physics of (geo)-materials, with a strong taste for numerical approaches. Interested applicants are invited to send a CV, a motivation letter and their transcripts to L. Brochard (laurent.brochard@enpc.fr) or A. Pouya (amade.pouya@enpc.fr) by **27 March 2020**.

Localization: Navier lab (https://www.navier-lab.fr) located at Ecole des Ponts ParisTech (6-8 avenue Blaise Pascal, 77455 Champs-sur-Marne, France)
Advisors: L. Brochard (laurent.brochard@enpc.fr) and A. Pouya (amade.pouya@enpc.fr)
Duration: 3 years, starting in Fall 2020
Funding: application for funding will be submitted in the framework of the call for grants of the Agence nationale pour gestion des déchets radioactifs. Following the eligibility rules of ANDRA, applicants must be **26 years old or less on October 1st 2020 and be citizen of the European Union**.

---

[2] Brochard et al. (2012) Journal of the Mechanics and Physics of Solids, 60(4), 606–622. http://doi.org/10.1016/j.jmps.2012.01.001
[3] Brochard et al. (2020) Revisiting thermo-poro-mechanics under adsorption: Formulation without assuming Gibbs-Duhem equation, under revision
[4] Ouraga (2017) Modélisation de la fracturation naturelle des sédiments: impacts sur la modélisation de bassin. PhD thesis ENPC.
[5] Disroc (2016) A Finite Element code for modelling coupled THMC phenomena in porous fractured media. Fracsima, www.fracsima.com
[6] Vo (2017) Modélisation Numérique et Analytique de la Fissuration de séchage des Sols Argileux. PhD thesis ENPC.
[7] Jung et al. (2020) Fracture Closure Mechanisms during Flowback from Hydraulic Fracture Networks, in preparation.