

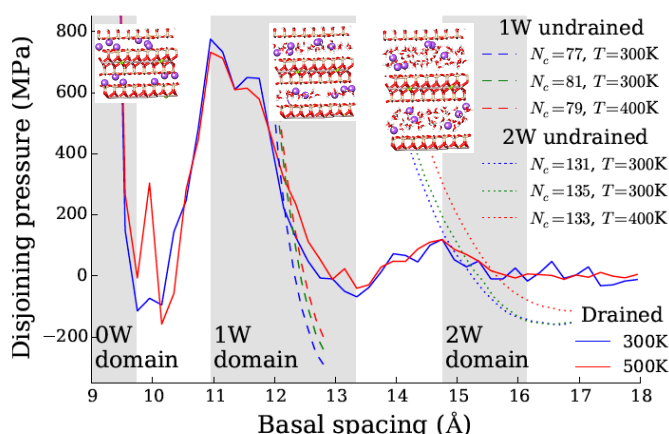
Context

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 simulation¹



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 CO_x in conditions corresponding to geological storage.

Poromechanical formulation

Taking into account adsorption in poromechanics is an active topic of research, which is not limited to claystone². Recent advances make it possible to take into account quantitatively the effect of bound water and its 6 moduli³. The practical implementation of the extended poromechanics is rather simple because the structure of the constitutive equations remains the same as in usual poromechanics 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 CO_x (from the literature or from ANDRA) will be considered.

We propose to set up a numerical implementation of this poromechanical model base on Disroc⁴. 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 reservoirs⁵, desiccation cracking of soils⁶, crack propagation under the effect of fluid injection⁷. 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.

Modeling of the behavior of a fractured porous medium submitted to gas pressurization

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

Context

In the context of the Cigéo project, the excavation of underground galleries in the Callovo-Oxfordian claystone induces a network of fractures around the excavated zone. This fracturing exhibits a typical profile of propagation in mixed I/II mode, which originates from the instantaneous discharge of the claystone after excavation. The topology and spatial extent of the induced network of fractures has been widely studied by ANDRA¹ around the excavations of the Laboratoire Souterrain de Meuse/Haute-Marne (LSMHM). Over long time, this network of fractures is expected to experience additional loadings by gas (mostly H₂) originating from the corrosion of metals used in the envelop of nuclear waste packages and from water radiolysis. The accumulation of these gases induces a pressurization that can affect the fractured zone. ANDRA has been investigating the risks associated with gas pressurization since 2003. In particular, gas-fracturing tests have been performed in a vertical well drilled from the surface and in wells drilled from the LSMHM.

The goal of this PhD project is to set up a numerical simulation tool able to model and simulate the mechanical response of a fractured porous medium submitted to gas pressurization while taking into account the peculiar thermo-hydro-mechanical (THM) couplings of claystone. The project is organized in three parts: 1- set up of the numerical tool, 2- numerical study under THM loadings with gas pressurization, and 3- confrontation experience-simulation.

Set up of the numerical simulation

We propose to set up the numerical simulation based on Disroc². Disroc is a finite element code dedicated in particular to the simulation of the fractured media. Cracking is accounted for by cohesive zone models, which are well adapted to the modeling of brittle and quasi-brittle media. These models avoid the main issues of Griffith models: they do not exhibit stress singularities at crack tips, and they can model both crack initiation and crack propagation. Disroc has already been used for the study of fracturing in several PhD and research projects in various labs including Navier lab. In particular, the propagation of fracture under THM couplings raises specific questions that have been addressed in the PhD thesis of Z. Ouraga³ dedicated to the natural fracturing of sedimentary formations (oil and gas reservoirs), and of T. D. Vo⁴ dedicated to the desiccation cracking of soils. A more recent research work⁵ investigated the propagation of fractures under the effect of a fluid injection (cf. figure).

The study of fracturing due to gas pressurization requires extending these works, dedicated to the case of a single incompressible fluid, to the case of a multi-phase fluid (liquid + gas) in an unsaturated medium. Recent researches at Navier lab make it possible to take into account quantitatively the effects of adsorption associated with bound water thanks to rigorous thermodynamics formulations of the poro-mechanics under adsorption^{6,7}. The numerical modeling proposed in this work will aim at integrating these new formulations. The

¹ Armand et al. (2014) Rock Mech. Rock Eng., 47, 21-41. doi:10.1007/s00603-012-0339-6.

² Ouraga (2017) Modélisation de la fracturation naturelle des sédiments: impacts sur la modélisation de bassin. PhD thesis ENPC.

³ Disroc (2016) A Finite Element code for modelling coupled THMC phenomena in porous fractured media. Fracsima, www.fracsima.com

⁴ Vo (2017) Modélisation Numérique et Analytique de la Fissuration de séchage des Sols Argileux. PhD thesis ENPC.

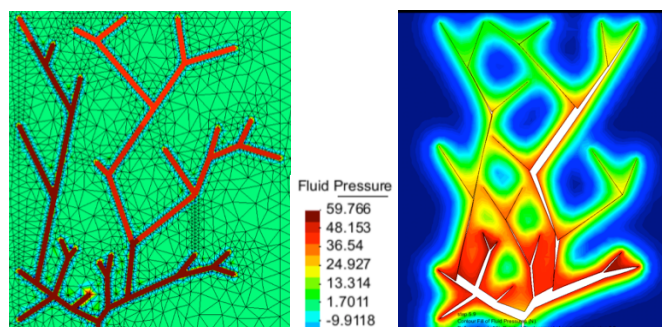
⁵ Jung et al. (2020) Fracture Closure Mechanisms during Flowback from Hydraulic Fracture Networks, in preparation.

⁶ 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>

⁷ Brochard et al. (2020) Revisiting thermo-poro-mechanics under adsorption: Formulation without assuming Gibbs-Duhem equation, under revision

implementation of these new poro-mechanical formulations in Disroc is rather simple (analytical formulation with the same structure as usual poro-mechanics).

Figure: Explicit modeling of the fractures induced by the injection of a pressurized fluid in a porous medium



Numerical study under THM loadings with gas pressurization

The parameters of the numerical tool will be calibrated so as to reproduce the behavior of the Callovo-Oxfordian claystone. In this respect, various experimental results available in the literature or obtained in other ANDRA projects will be considered. The behaviors of the non-adsorbed fluids (gas, free water) will be accounted for with usual models (ideal gas, incompressible, or empirical equation of states if these two limit cases prove inappropriate in the range of temperatures-pressures of interest). The behavior of the bound water will be obtained by crossing experimental data of the THM couplings and molecular simulation data available in the literature⁸.

The numerical tool will then be applied to various simple cases in order to evaluate the main factors influencing the gas breakthrough. Special attention will be dedicated to the role of THM couplings specific to claystone (notably: swelling/shrinkage and thermal pressurization).

Confrontation experience-simulation

In order to evaluate the numerical model, a confrontation with experiment is necessary. In agreement with ANDRA, the numerical model will be used to simulate the gas-fracturing tests performed at LSMHM or other lab tests performed for ANDRA during this PhD. The 3D aspects will be accounted for with the future version of Disroc that shall be released during this PhD.

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**.

⁸ Honorio et al. (2017) Langmuir, 33(44), 12766–12776. <http://doi.org/10.1021/acs.langmuir.7b03198>