



## CNRS PhD position at GeoResources laboratory (Nancy, France)

### Investigation of hydromechanical and electrokinetic couplings during gas migration in saturated clayey rock at mesoscopic scales

**Background and Objectives:** In a geological repository for radioactive waste, corrosion of ferrous materials under anoxic conditions, associated with radioactive decay of waste and water radiolysis, will lead to the formation of hydrogen. A full understanding of the migration behaviour of this gas is of fundamental importance for the reliability of scenarios predicting the long-term evolution of such a repository. If the rate of gas production exceeds the rate of gas diffusion into the pores of the host rock, a distinct gas phase will form. Capillary forces opposing the movement of the gas will cause the pressure to increase to a critical value beyond which it can penetrate into the surrounding material and move through advective processes. However, different mechanisms specific to clayey rocks and their nanoporous nature could influence these viscous capillary flows.

First of all, due to the high pressures generated, the percolation of gas generates an expansion of the percolating paths, which can lead to a localized displacement of water away from these paths, under the effect of compression of the clay matrix [1]. These phenomena of opening of the percolating paths (microcracking) in turn lead to damage and degradation of the mechanical properties of the rock. If the pressure continues to increase, tension fractures develop in a similar manner to those observed in hydraulic fracturing. At the same time, in clayey environments such as Callovo-Oxfordian clay (COx) the pore water contains dissolved ions and thus forms an electrolyte. Due to the electrical charges present in the clay sheets the concentration density of the ions near the solid/liquid interfaces becomes inhomogeneous and the electrolyte is no longer electrically neutral (electrical double layer). The flows are in this case more complex since couplings occur between the dynamics of the solvent and that of the ions. Indeed, when the fluid is subjected to an electric field, although the solvent is neutral, a hydraulic flow is observed. This mechanism, called electro-osmosis, is particularly important in the context of radioactive waste disposal because of the introduction of ionic radionuclides into the geological layer in addition to the ions naturally dissolved in the pore water.

The objective of this thesis is to propose mesoscopic models capable of taking into account HydroMechanical (HM) and ElectroKinetic (EK) couplings when simulating flow and transport in large representative elemental volumes (REVs) typically out of reach of molecular methods. This will allow quantitative analyses of the simultaneous effects of real clay morphology and HM and EK couplings on transport properties.

**Scientific content:** Numerical simulations of drainage will be carried out on high-resolution 3D images (MET and FIB-SEM images) of the CO<sub>x</sub> argillite. Two numerical methods, Lattice Boltzmann (LBM) and Smooth Hydrodynamics Particle (SPH), whose codes were developed in previous projects will be used for this purpose. The results obtained will be validated on the basis of experimental tests from the literature or carried out in the laboratory.

Hydromechanical coupling: We will first study the consideration of geomechanical couplings to reproduce certain characteristics of long-term gas behaviour, and more particularly the development of expansion paths with gas migration through localised fractures. Several strategies with different levels of complexity to describe these poromechanical effects will be considered and implemented in the LB and SPH models. The results obtained will be compared and regime diagrams will be established in order to evaluate the most relevant approach according to the hydrodynamic constraints (e.g., maximum gas pressure) and the degree of accuracy required. The SPH model will be based on the representation of the clay medium by a linear elastic solid matrix with isolated rigid inclusions, while a poromechanical damage model will describe the degradation of mechanical properties under local stress [3]. This model will be enriched by taking into account plasticity. At the level of the LBM model [4], two strategies will be considered. Firstly, immersed boundary conditions or interpolated boundary conditions [2] will be implemented in the model in order to make the geometry evolve at the pore scale under the effect of increasing pore pressure. A second, more complex and therefore more expensive approach will consist in coupling the LBM model with the discrete element method (LBM-DEM) in order to accurately describe the mechanical behaviour of the solid skeleton and the creation of new percolating paths. The DEM will model the solid particle phase by treating each particle as a separate rigid body while the LBM will solve Navier Stokes' incompressible equations. The interaction at the fluid/solid interface will be solved by an immersed boundary condition scheme.

Electrokinetic coupling: For the simulation of electrokinetic couplings, including electroosmosis, we will focus on LBM type methods that have been already used with success [5] but only for simplified geometries where analytical solutions exist and for saturated conditions. For an electrolyte confined in a charged porous medium with mesoscopic pore sizes, the electrokinetic couplings are incorporated by adding to the hydrodynamics equation a local force term to which the fluid is subjected due to the electrostatic shielding of surface charges by dissolved ions. This coupling term is therefore dependent on the dynamics of the ions which is in turn coupled to the fluid dynamics through advection. Finally, the ions are subjected to the local electric field which is calculated from the electrostatic potential that satisfies Poisson's equation. In summary, the dynamics of the system obeys a system of coupled equations consisting of the Navier-Stokes equation for the solvent, the Nernst-Planck (diffusion-advection-migration) equations for the ions and the Poisson equation for the electrostatic potential. It is important to remember that this description of the coupled dynamics of the ions and the solvent corresponds to mesoscopic pores ( $d > 2$  nm) where the hydrodynamics equations are valid and where the molecular aspects of the ions such as solvation effects or excluded volume type effects are negligible.

We plan to use here a so-called "integral" approach [6] which solves all the dynamics by the LBM method but which has been used for the moment only for 2D cases. This exclusive use of the LBM equations should allow an efficient parallelization of the numerical scheme, and thus access to large volumes. In practice, the implementation of the integral method generalized to the three-dimensional case will be carried out in the parallelized LB simulation code developed and maintained at the

GeoRessources laboratory. Technically, it is sufficient to solve not one but four LB equations with lower order velocity discretization (D3Q7) for ions and electrostatic potential than for hydrodynamics (D3Q19). Although the algorithm proposed here uses a single relaxation time for each of the equations, it is possible to generalize the method for the use of multiple relaxation times as in [4] to improve the overall stability of the method.

**Prerequisite:** The candidate must be a highly motivated and autonomous person with a recent university master's degree (or equivalent) in mechanics, reservoir engineering, applied mathematics, civil engineering or other relevant field. He or she must demonstrate a fundamental knowledge of the principles of fluid mechanics governing the behaviour of porous media. Experience in the development of numerical methods, in particular LBM methods would be an asset. The candidate should be fluent in English and French (or show a willingness to learn French).

**Funding:** The proposed thesis is funded by a CNRS doctoral contract and is part of a larger [NEEDS](#) project that aims to mobilize academic research on major nuclear-related issues.

This thesis project is funded for 3 years, ideally starting October 1st, 2020 (gross salary: ~ 2135€/month). This thesis work will be carried out within the [GeoRessources](#) laboratory (in the research team "Multiscale HydroGeoMechanics", University of Lorraine/CNRS) in Nancy, in collaboration with [LFCR](#) (Laboratoire des Fluides Complexes et leurs Réservoirs - UPPA/TOTAL/CNRS) and [IRSN](#) (Institut de Radioprotection et de Sécurité Nucléaire).

**Contacts and how to apply:** Candidates are invited to submit their CV, master's transcripts and cover letter here: <https://bit.ly/2W2NFhI>

Please also send your application to the emails below

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## References :

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