PhD thesis subject: Call for candidates.

Multiscale modelling of coupling between reactive transport of chemical species and geomechanical behaviour of rock reservoir: Application to geological storage of CO2.

Advisors :
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Context
The geological storage of CO2 coming from large industrial facilities has been studied in detail for the last several years as a solution against the greenhouse effect and climate change in a number of countries. It is considered as a complementary solution together with the research for the non pollutant or/and renewable energy sources. One of the available options is the injection of the supercritical CO2 in the saline aquifers. The idea of geological storage resides in various mechanisms of trapping coming into play progressively over time. In the short term the migration of CO2 is principally blocked by the impervious rock lying on the top of the aquifer. As time goes on, other mechanisms appear, in particular of geochemical nature, like the dissolution of CO2 in pore water, and finally the chemical reactions (dissolution and /or precipitation of rock minerals). These reactions can generate important and irreversible modifications of the hydrodynamical as well as mechanical properties of the reservoir. The long-term safety of the CO2 storage sites requires the understanding of the physicochemical processes related to the injection of the CO2 in the geological medium and their consequences, especially for the stability of the reservoir. These processes are still not completely known, in particular because of the complexity of natural systems, those are very often heterogeneous and multiscale, and also because of multiphysical couplings engendered by the CO2 injection.

Objective
The aim of the thesis is to develop a macroscopic model of reactive mass transport coupled with the poro-mechanical model of aquifer, and to define its domain of validity. The proposed study will focus on the long-term (and/or the far field) behaviour, when the physicochemical phenomena risk influencing the behaviour of the whole aquifer. The important objective of this work is to find the link between the microstructure of the material and the phenomena occurring at the microscopic scale, and the observed macroscopic behaviour. It will be possible as a result of the chosen modelling method (multiscale homogenization) and the laboratory experiments.

Methodology
The theoretical modelling by homogenization consists (classically) of three principal stages: i) Formulation of the problem at the local scale, ii) Homogenization properly speaking, and iii) Analysis of the obtained macroscopic problems. The phenomena that will be taken into account are: chemical reactions in competition (in the liquid phase and at the interfaces), mass transport mechanisms by advection and diffusion, as well as geomechanical effects resulting from the modification of the microstructure of the porous reservoir. The numerical computations of the parameters of the model using the codes Comsol Multiphysics (@LMGC) and ANSYS-FLUENT (@GM), are envisaged. The experiments of reactive percolation in the laboratory conditions will be carried out. The experimental conditions will be representative of the homogeneous dissolution taking place far from the injection well and at long duration. The mechanical properties will be measured before and after the flow and transport experiment by using the triaxial apparatus. The aim is to quantify the modifications induced by the dissolution. In the second phase, the similar experiments in the precipitation conditions will be performed. In parallel, the modifications of the microstructure will be measured by means of the X-ray microtomography (the resolution will vary from 1 to 10 microns). Finally, the fluid composition at the exit from the sample and the permeability will be measured during the experiment. It will enable us to know (at the scale of the sample) the rate of the dissolution (i.e. the flux of the dissolved or precipitated matter) and the modifications of the hydrodynamic properties. The whole set of data will be used to characterize the microstructure that is needed for homogenization, and also as a tool for validation of the macroscopic multiphysics model.

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