Master 2 internship proposal: Pore scale finite element modelling of calcite dissolution in caprock formation

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General context

According to The Intergovernmental Panel on Climate Change (IPCC) AR6 synthesis report: Climate Change 2023 [1] in global modeled pathways that limit global warming to $2\,°C$ or below, almost all electricity is supplied from zero or low-carbon sources in 2050, such as renewables or fossil fuels with CO_2 capture and storage (CCS). CCS in deep geological formations has consequently emerged as an important option to reduce greenhouse gas emissions and CCS facilities are continuing to grow in Europe.

The aim of LOCCO project to work on these actions to increase knowledge of the interaction between the CO_2 injected in geological storage reservoirs and the surrounding rocks, which should act as sealing barrier, to the CO_2 migration and leakage, and guarantee long-term storage security. The purpose is to improve performance of the technologies that are currently adopted in CO_2 geological sequestration, investigating the role of coupled processes occurring within the geological reservoir and at its interface with the so-called tight caprock. The analysis is here centered on aquifer rock reservoirs, which can store large amounts of CO_2 (the International Energy Agency, IEA, estimates that saline aquifers have the capacity to store over 10,000 Gt of CO_2, say enough room to hold over 100 years worth of emissions from all global stationary sources) and are widespread in Europe and in France. The key coupled hydro-chemo-mechanical phenomena, which could be detrimental to the sealing potential and structural integrity of clay-rich caprock, will be studied in the laboratory and predicted through new modeling and numerical tools, on which this internship offer focuses.

To be more specific, in geological sequestration, CO_2 is injected in liquid form (low temperature, modest-to-high pressures), but it transforms into a supercritical fluid ($scCO_2$) as it is injected and warms to the temperature of the formation. Having density lower than the aqueous brine, initially saturating the reservoir rock, $scCO_2$ tends to buoy through it, in continuous contact with the brine, and to accumulate below the caprock. In particular, four zones are identified: a zone I, fully saturated by $scCO_2$, in the close vicinity of the injection well, a zone II, characterized by the presence of a two-phase mixture of $scCO_2$ and brine with possibly buffered pH, a zone III fully saturated with an aqueous solution acidified by CO_2 and a zone IV unaffected by CO_2 injection, see figure 1. In each of this zone, the degradation of the caprock is driven by different mechanisms.

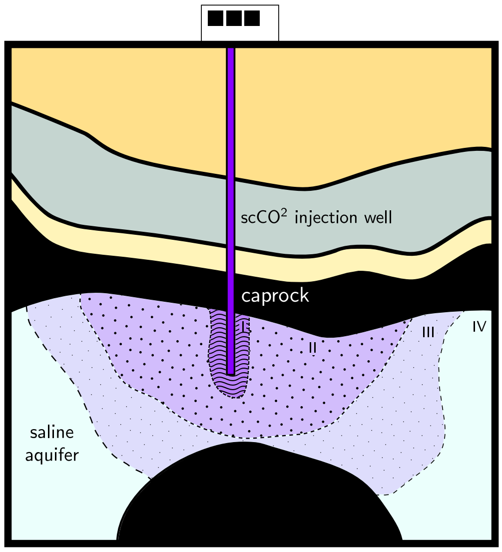

Figure 1 – Schematic representation of the different zones in the saline aquifer, modified after [2]

Work Program

This internship focuses on the degradation mechanisms occuring in zone III. In this zone, diffusive-reactive processes take place which tend to acidify the solution, in contact with the caprock, and whose pH depends on the CO_2 saturation. As a consequence, carbonic acid can penetrate the caprock, mainly *via* a diffusion process and alterate its microstructure due to calcite dissolution, resulting in modifications of its diffusion and hydraulic properties, possibly favoring the CO_2 penetration, and then eventually involving a positive feedback ("snow-ball effect") that may lead to CO_2 leakage. The main objective of this internship is to pave the way for a further PhD program that will focuses on this topic, by developing and implementing a model of this diffusion/dissolution phenomena, at the pore scale, using Finite Element Method. To achieve this work, the intern will first perform a litterature review, especially in order to identify several modelling approaches of pore scale dissolution. A particular attention will be devoted to the description of the evolving fluid-solid interface and a detailed comparison between level-set and phase-field approaches of this problematic, in a finite element context, will be necessary to choose the most suitable one. This first step will lead to the formulation of an IBVP (initial and boundary value problem) in which we represent the fluid flow in a reactive porous media, and where the solid fluid interface is captured by an implicit method. In order to solve this problem, the candidate will then use the open source finite element code FEniCSx [3]. Finaly, guided by existing formal homogenisation results [4-6] the intern will prepare the interpretation of the numerical results in terms of estimation of permeability and diffusivity.

Main outcomes: The main outcomes of this work will be the formulation and implementation of a dissolution model at the pore scale, which will paves the way for the development of a hierarchical two-scale formulation of the problem as intended by the ANR project "LOCCO" through an upcoming PhD program.

Applications and additional informations

Applications - Detailed CV including bachelor and master transcripts and cover letter are to be sent to Quentin Rousseau (✉) and Pierre Besuelle (✉). Recommandation letters are welcome but not mandatory.

Profile - Basic knowledge in continuum and fluid mechanics, finite element method, and scientific programming (e.g. Python, numpy, matplotlib) are required to achieve this project.

Facilities - The internship will start in Febuary, for a duration of 5 months. It will take place at the Laboratoire 3SR in Grenoble (France). The intern will be part of the Geomechanics group (website) which is leading cutting edge investigations concerning the mechanics of geomaterials at various scales, and considering the associated multiphysical couplings.

Remuneration - The recruited candidate will be gratified according to the regulations in force.

PhD opportunities - In the context of ANR LOCCO, a PhD grant in complete continuation with this proposal is already fully secured. This constitutes a solid opportunity for the selected intern to pursue as PhD candidate on a closely related topic, starting on Fall 2026.

References

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