PhD position at Institut de recherche en Génie Civil et Mécanique[1] (GeM), Ecole Centrale de Nantes & Urban and Environmental Engineering[2] (UEE), Université de Liège

"Modeling hydro-chemo-mechanical phenomena in CO_2 geological sequestration"

Responsibles of the research project:
Giulio Sciarra[1], Frédéric Collin[2], Siddhartha H. Ommi[1]

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) in deep geological formations**. CCS has consequently emerged as an important option to reduce greenhouse gas emissions and CCS facilities are continuing to grow in Europe. However, global rates of CCS deployment are far below those envisaged to limit global warming. It is the aim of **LOCCO project** ("hydro-chemo-mechanical LOCalization phenomena in CO_2 geological sequestration" financed by ANR – *Agènce Nationale de la Recherche* – in France) 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.

In geological sequestration, CO_2 is injected in liquid form, but it transforms into a supercritical fluid ($scCO_2$). 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 therefore to accumulate below the caprock. Different zones within the aquifer host rock at different distances from the injection well can be identified, which are differently affected by the $scCO_2$ concentration, see Figure 1; in particular 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 [2]. In the worst-case scenarios, the solution stored in zones I, II and III could be significantly acidified with respect to the almost neutral characteristics of natural brine.

Project overview

Significant efforts in the literature have been devoted to understanding the response of reservoir rock to CO_2 injection; however, considerably fewer results address the direct interaction between the acidified solution stored in the aquifer and the caprock. While chemo-hydrodynamic pattern formation has been

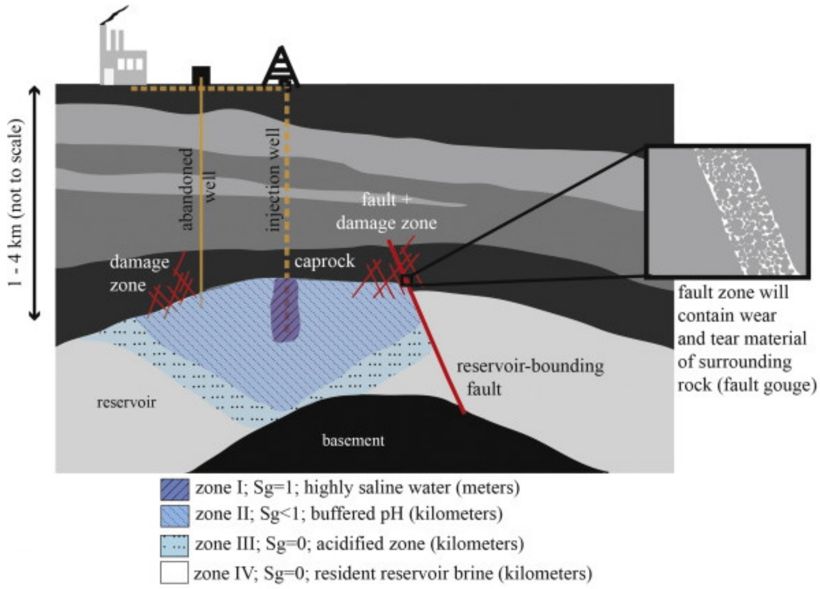

Figure 1: Characteristic zones around the CO_2 injection well, see [2].

extensively studied in porous media, for instance in polymers, its implications on the deformation and structural integrity of solid porous structure remain poorly understood.

For what concerns CCS operations, the following scenarios could be considered as the most representative of hydro-chemo-mechanical interactions between the acidic brine solution and the caprock. S1) The pressure of the scCO_2 at the top of the reservoir is lower than the gas-entry pressure of the caprock. As a consequence, the CO_2 cannot flow through the caprock but cations diffuse through it. **Geo-chemical alteration of minerals prone to acid attack**, can occur because of the chemical disequilibrium between the brine, saturating the clayey rock, and the acidified solution. S2) **Pre-existing fracture network/faults**, having gas-entry pressure lower than the scCO_2 pressure and intrinsic permeability higher than that of the surrounding clay-rich rock (typically two order of magnitude), act **as flow conduits for the acidified solution**. In this case, the scCO_2 bypasses to a large extent the rock matrix by flowing through the fracture paths. S3) The pressure of the scCO_2 at the reservoir top exceeds the gas-entry pressure of the caprock matrix. In this case, the CO_2 penetrates through the caprock via a **drainage process** (a non-wetting fluid displacing a wetting one).

Which scenario prevails depends on the characteristic time scales associated with the above processes. These can be characterized and quantified using a suitable poro-hydro-chemo-mechanical model parameterized by an appropriate set of dimensionless numbers (including Péclet number, Damköhler number, capillary number and viscosity ratio). The project focuses on formulating this coupled model and implementing it numerically, thus paving way towards practical estimates of safe storage capacities of CO_2 in geological reservoirs. Moreover, while scenario S2 might intrinsically mean a non-homogeneous transport of scCO_2 across the caprock via fractured pathways, S1 & S3 might present flow regimes with both homogeneous transport and transition to non-homogeneous pathways (for instance **worm-holing** in S1 and **viscous fingering** in S3). Associating such pattern-forming unstable regimes to the magnitude of the various dimensionless numbers would also be of special interest.

Objectives and scientific program

The objectives of the research activity will be the rigorous **formulation, at a continuum-scale,** of a suitable poro hydro-chemo-mechanical model to describe the above-mentioned phenomena and the **numerical implementation** of the same, within the **LAGAMINE** Finite Element code (mainly developed at UEE).

In particular the scientific program consists of the following tasks:

- **Modeling dissolution and precipitation of carbonate minerals** within the caprock driven by diffusive and/or advective transport of cations, which can dampen or enhance visco-capillary fingering and alter the micro-structure of the solid skeleton;
- **Modeling two-phase visco-capillary flow**, as an extension to the phase field approach to partial saturation in porous media proposed in [3, 4, 5];
- **Modeling alteration of stiffness and strength properties of the caprock** by dissolution/precipitation, which could trigger deformation bands and localized strain depending on the loading condition and the material properties;
- **Implementing the model within LAGAMINE FE code** by updating existing subroutine on chemo-mechanical physics, and taking advantage of a subroutine implementing the phase field approach to partial saturation, which is currently under development.
- **Simulating FE test-cases** to reproduce laboratory-scale conditions. These results will inform on the relevant scaling laws to be used within a parallel experimental research activity carried out within the LOCCO project. This provides an unique opportunity to have a dialogue between modeling philosophies and experimental inferences.

Application and additional information

Application - Detailed CV including transcript of records of current master formation and cover letter are to be sent to Giulio Sciarra (giulio.sciarra@ec-nantes.fr), Frédéric Collin (F.Collin@uliege.be), and Siddhartha H. Ommi (siddhartha-harsha.ommi@ec-nantes.fr). Recommendation letters are also required.

Profile - A solid background in continuum mechanics and computational mechanics is also required. Advanced knowledge in scientific programming is also requested (e.g. Python, Matlab, possibly FORTRAN).

The PhD contract will start in September 2026, for a duration of 36 months. It will take place at the GeM, Ecole Centrale de Nantes (France) and UEE, Université de Liège (Belgium) within the framework of a cotutored PhD thesis (*thèse en cotutelle*).

References

[1] Climate Change 2023 Synthesis Report. Contribution of Working Groups I, II and III to the 6th Assessment Report of the Intergovernmental Panel on Climate Change, doi: 10.59327/IPCC/AR6-9789291691647

[2] Rohmer, J. et al. 2016, Mechano-chemical interactions in sedimentary rocks in the context of CO_2 storage: weak acid, weak effects?, Earth-Science Reviews 157, 86-110.

[3] Sciarra, G. 2016, Phase field modeling of partially saturated deformable porous media. Journal of Mechanics Physics of Solids, 94, 230-256.

[4] Ommi, S. H., Sciarra, G., & Kotronis, P. 2022, A phase field model for partially saturated geomaterials describing fluid–fluid displacements. Part I: The model and one-dimensional analysis. Advances in Water Resources, 164, 104170.

[5] Ommi, S. H., Sciarra, G., & Kotronis, P. 2022, A phase field model for partially saturated geomaterials describing fluid–fluid displacements, Part II: Stability analysis and two-dimensional simulations. Advances in Water Resources, 164, 104201.