Experimental Investigation of the Coupled THMC Response of the Caprock to CO₂ Injection in a Pilot Test Site

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Objectives

Carbon capture, utilization, and storage (CCUS) is crucial for mitigating industrial greenhouse gas emissions. Geological sequestration in sedimentary basins, particularly within low-permeability argillaceous caprocks such as the Opalinus Clay Formation (OCF), offers secure, longterm CO₂ storage. This research explores coupled thermal, hydrological, mechanical, and chemical (THMC) processes in OCF under sustained CO₂ injection. Utilizing experimental data from the Mont Terri Underground Rock Laboratory (MTURL), the study aims to develop robust predictive models for assessing caprock stability and informing effective monitoring strategies.

Research Advancements

Doctoral research in the current phase encompasses two primary domains: geochemical and geomechanical studies. This research significantly advances multi-scale reactive transport modelling to investigate the geochemical response of the OCF to CO₂ injection. Initial 0D geochemical models using PHREEQC [1] and CHESS [2] software provided foundational insights, facilitating the selection of the Thermo-Chimie database [3] for subsequent simulations. These models evolved into more comprehensive 1D reactive transport simulations with HYTEC software [4], successfully calibrating porewater chemistry against data from the MTURL [5].

Two distinct 2D reactive transport models were subsequently developed using HYTEC. The first aligns precisely with the CO₂ Long-Term Periodic Injection Experiment (CO₂LPIE) at Mont Terri [6], providing detailed insights into carbonate mineral dissolution and re-precipitation dynamics. Benchmarking conducted collaboratively with international research institutions initially identified pH as a critical indicator, showing geochemical perturbations confined to approximately one metre around the CO₂ injection point over 20 years. These outcomes have directly informed the optimal placement of monitoring wells.

The second 2D models specifically addresses lithofacies-dependent hydrogeochemical responses, comparing shaly, sandy, and carbonate-rich sandy facies under CO₂ injection. Results demonstrated significant variability in mineral reactivity: minimal alterations in shaly facies confirmed their suitability as effective caprock, while the carbonate-rich sandy facies showed pronounced dissolution and precipitation reactions. Intermediate geochemical responses were observed in sandy facies. These findings underscore the critical role of lithofacies heterogeneity, reinforcing the need for facies-specific evaluations within integrated THMC modelling frameworks.

Ongoing Research Activities

Reactive transport modelling studies are currently underway, utilizing experimental data from the CO₂ injection and Direct Observation of Fluid Propagation (CS-D) experiment conducted previously at MTURL [7]. This experiment investigates the fundamental chemical and physical processes influencing CO2 migration within a fault damage zone, its interaction with surrounding undisturbed rock, and how fault permeability is affected by injecting CO₂ into the main fault crossing the shaly facies of the OCF. The ongoing simulations will be carefully calibrated using these experimental findings to further clarify these critical mechanisms. In parallel, further research will focus on the second primary domain of the doctoral project, geomechanical studies, and its coupling with the previously developed geochemical framework. Following this THMC coupling, mesoscale simulations incorporating both reservoir and caprock characteristics will be performed to predict caprock integrity under realistic CO₂ storage

- $\hbox{[1] Parkhurst and Appelo, 2013, USGS, Technical Report.}\\$
- [2] Van Der Lee and De Windt, 2002, LHM/RD/02/13.
- [3] Giffaut et al., 2014, Applied Geochemistry, 49, 225-236.
- [4] Van der Lee et al., 2003, Comp. & Geosc., 29, 265-275.
- [5] Koç et al., 2024, EGU24-3952. Abstract.
- [6] Rebscher et al., 2019, ECCSEL Workshop, Abstract.
- [7] Zappone et al., 2021, Solid Earth, 12, 319-343.