

Two phase simulation and Bayesian inversion for CO₂ storage in porous media

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Introduction and Motivation

CO₂ sequestration is a complex multiphysics process, in which multiphase multicomponent flows play critical role. The fact that the CO₂ should be stored for many thousands of years implies that full scale experiments are not possible, and computer simulation is the main approach for exploring the feasibility of different CO₂ storage options. Various risks exist in CO₂ sequestration, the most important being (i) CO₂ leakage through cap-rock failure, faults, abandoned wells, (ii) Brine displacement and infiltration into drinking water aquifers. Quantification of the risks and uncertainties is of ultimate importance for the decision makers when evaluating the storage approaches.

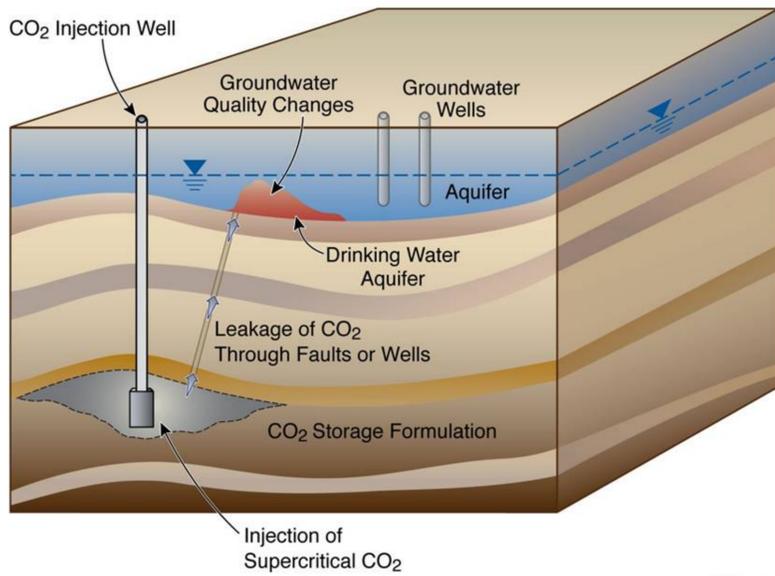


Figure 1: Picture of ESD

Parameters are affected by uncertainty (because they are not perfectly known or because they are intrinsically variable). The general objective of our project is to devise effective ways to include, treat and reduce uncertainty in a mathematical model, more precisely to derive, calibrate and validate predictive macroscopic models that incorporates the relevant phenomena. In this work we simulate leakage scenario of CO₂ storage, and we estimate the parameters of the macro scale model.

Physical Hypothesis and Model

- 2 phases: brine and CO₂
- Darcy's law for the velocity of each phase
- The capillary pressure between liquid pressure and CO₂ pressure is a non linear function of the liquid saturation $p_c(S_w) = p_n - p_w$
- Phases occupy the entire pore space: $s_w + s_n = 1$
- Mass conservation for each phase

$$\phi \partial_t (\rho_w S_w) + \text{div} (\rho_w \mathbf{V}_w) = Q^w,$$

$$\phi \partial_t (\rho_n S_n) + \text{div} (\rho_n \mathbf{V}_n) = Q^n.$$

ϕ = porosity
 ρ_α = density of the α phase
 s_α = saturation of the α phase

p_α = pressure of the α phase
 \mathbf{V}_α = Darcy's law for the velocity
 Q^α = source term

Numerical simulation: Leakage of CO₂ from the aquifer through an abandoned well

CO₂ is injected into an aquifer, spreads within the aquifer and upon reaching a leaky well, rises up to a shallower aquifer. A quantification of the leakage rate which depends on the pressure build-up in the aquifer due to injection and on the plume evolution is the goal of the simulation (Figure 2).

The aquifers are initially filled with brine ($s_n = 0$). The initial conditions in the domain include a hydrostatic pressure distribution which is dependent on the brine density. The lateral boundary conditions are constant Dirichlet conditions and equal to the initial conditions. All other boundaries are no-flow boundaries. CO₂ is injected at a constant rate of 8.87 kg/s and the simulation time is 1000 days.

Figure 3 show the 2D simulation of the benchmark (with in-house code). Figure 4 show the 3D simulation of the benchmark with DuMuX open source [3]. Figure 5 show the CO₂ leakage through the leaky well as a function of time. This is defined here as the CO₂ mass flow at midway between top and bottom aquifers divided by the injection rate, in percent.

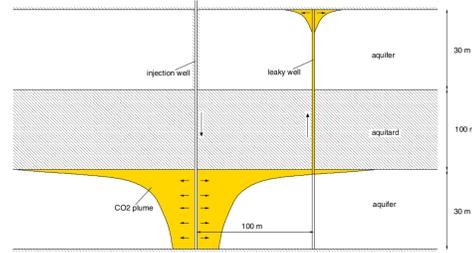


Figure 2: Scenario of the Benchmark [1, 2]

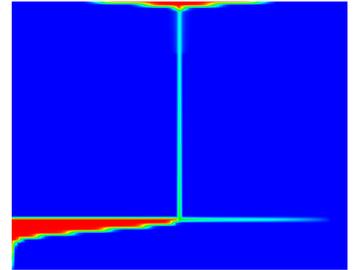


Figure 3: 2D simulation of the benchmark

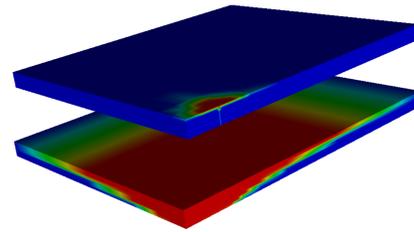


Figure 4: 3D simulation of the benchmark

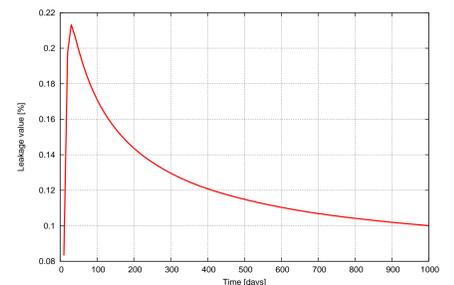


Figure 5: CO₂ leakage through the leaky well as a function of time

Bayesian Inversion

The inverse problems can be stated as: Given data D and forward model \mathcal{F} , find parameters θ . Bayes' theorem prescribes how to incorporate a priori data and measurements into the model.

$$P(\theta|D) = \frac{P(D|\theta) P(\theta)}{P(D)} \quad \text{Bayes formula}$$

$$P(D) = \int P(D|\theta) P(\theta) d\theta$$

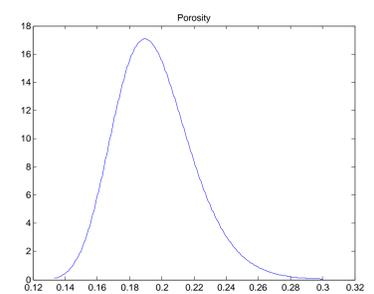
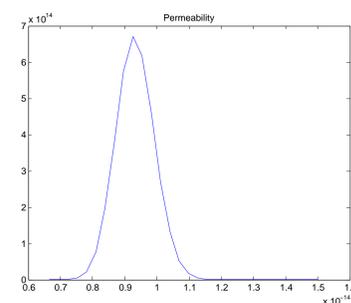
$$D = \mathcal{F}(\theta) + \epsilon; \quad \epsilon_i \sim \mathcal{N}(0, \sigma^2) \text{ where } \epsilon = \text{noise}$$

The Bayesian inversion estimates probability distribution of θ . In this case the porosity and the permeability.

- The data are synthetic data with parameters proposed by the benchmark
- $P(\theta)$: **Prior distribution** for the parameter θ can be assumed using available information
- $P(D|\theta)$: **The Likelihood**

Parameter estimation

The porosity and the permeability has been considered as parameters. The a posteriori of both are computed. The effective porosity and permeability is found to be very close to the reference.



References

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- [2] Nordbotten, J., Celia, M., Bachu, S., 2005a. Injection and Storage of CO₂ in Deep Saline Aquifers: Analytical Solution for CO₂ Plume Evolution During Injection. Transport in Porous Media 58(3), 339–360.
- [3] DuMuX web-page: <http://www.dumux.org>

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