Abstract

The storage of carbon dioxide plays a fundamental role in our global effort to reduce the atmospheric concentration of greenhouse gases (GHG) and achieve our long-term climate goals (Metz 2005). Regardless of the choice of capture method, in the end greenhouse gases must be stored safely and permanently. The pore space in sedimentary rocks is considered more than enough to store all the CO$_2$ that we could possibly want to remove from the air (Kramer 2020), making geological sequestration a promising carbon storage technology.

Geological sequestration involves the injection of CO$_2$ in either (dissolved) gas, liquid, or supercritical phase, into the pore space of subsurface rock formations, such as abandoned oil and gas reservoirs and saline aquifers. Once there, CO$_2$ can become trapped due to a series of physical and/or chemical mechanisms (Zhang 2014). Some of these mechanisms relate directly to the pore scale, such as structural, residual, and mineral storage. Structural storage happens when CO$_2$ is injected as a less-dense-than-water phase under a low-permeability caprock that prevents the lighter fluid from floating up. In residual storage, also known as “capillary trapping”, CO$_2$ droplets or bubbles become (physically) trapped due to the capillary forces that dominate in the constricted space of the pore channels. The most stable storage mechanism is the mineralization of CO$_2$ that (chemically) reacts with the rock surface to form solid carbonate minerals. This process takes longer than the others because it requires that CO$_2$ first dissolves in water to form carbonic acid, but this acid formation can be accelerated by creating the CO$_2$-rich solution before underground injection (Snæbjörnsdóttir 2020).

To study these storage mechanisms, a robust framework for the simulation of fluid flow at the pore scale is required. There are many options to be considered, such as finite-element, finite-volume, lattice Boltzmann, density-functional and network models, each one with its associated computational costs and applicability (Meakin 2009, Saxena 2017). What all these models have in common is the need for an accurate description of the pore scale geometry of the host rock. For that reason, three-dimensional digital images acquired via x-ray computed micro-tomography (µCT) have become ubiquitous as the geometrical basis for the realization of pore scale flow simulations, in a field called “Digital Rock Physics” (Andrä 2013).
In this work, we present the application of a cloud-based, pore-scale flow simulator to the study of CO$_2$ storage in geological formations. Cloud computing is a relatively new computing paradigm prized for its elasticity, scalability, availability, and performance (Mell 2011) that allows shifting CAPEX to OPEX costs under a “as a service” charging model. The prototype technology can be summarized as follows: a cloud storage space that stores the microtomography images, a REST API that allows the submission of data processing and flow simulation jobs and a web-based graphical user interface that facilitates the interaction with all the other components.

We used such tool to perform single-phase flow simulations using a capillary network model and calculate the permeability of several sedimentary rocks with a diverse distribution of geometries and morphologies (Neumann 2021). The ability to compute the permeability of a caprock layer is fundamental to assess the effectiveness of structural storage in each scenario. We have then extended such simulation tool to account for multi-phase flow phenomena that is relevant for the study of the physical mechanisms behind residual storage. We perform a sensitivity analysis with respect to multiple fluid parameters, such as viscosity, interfacial tension, contact angle, pressure, and temperature, and quantify their influence on the infiltration and retention of CO$_2$ inside a capillary network that is representative of an actual rock.

We also explore the possibility of experimental validation, where applicable, using a combination of a Si/SiO$_2$-based rock-on-a-chip platform, optical imaging, and spectroscopy techniques to monitor the flow and imprisonment of CO$_2$-laden fluids in constricted geometries (Tirapu-Azpizroz 2022). Our final goal is to reproduce both computationally and experimentally the chemical reaction dynamics behind mineral storage and propose material additives that can make geological storage faster, safer, and cheaper.

References

Metz, Bert, et al. IPCC special report on carbon dioxide capture and storage. Cambridge: Cambridge University


*Keywords*: cloud computing; flow simulation; pore-scale; capillary network; digital rocks; carbon dioxide.