May 23 - 26, 2022

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IEEE MICROELECTRONICS DESIGN & TEST SYMPOSIUM

2022 IEEE MDTS
The 31st Microelectronics Design and Test Symposium
May 23-26, 2022
Virtual meeting

On-chip analysis of fluid flow for applications in carbon dioxide trapping

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Carbon dioxide capture and storage into underground geological formations is a promising route to reduce emissions into the atmosphere and limit global warming. Geo-sequestration involves the injection of carbon laden solutions directly into the pore space of subsurface rock formations, such as saline aquifers and abandoned oil reservoirs in sedimentary rocks, saline formations, or abandoned oil fields. Accelerated discovery of low-cost materials and scalable processes through AI-driven design and cloud-based computational simulations can help identify injection processes and additives capable of enhancing CO_2 sequestration. More scientific research is still needed to understand how the pore structure and material properties of the rock matrix influence the extent to which pressurized fluids can be injected, permeate, and form stable carbonate minerals within the pore network.

Our research focuses on studying the fundamental mechanics of pore infiltration at micro- and nanoscopic scales to develop a comprehensive model of carbon dioxide sequestration within geological pore networks. We model the rock pore space as a network of capillaries with spatially varying radii to match the local geometry, and within each capillary the flow rate is modelled as laminar flow. This fined-grained capillary network representation is extracted from high-resolution X-ray microtomography images of suitable rocks and allows for both single- and two-phase flow simulations of fluid injection into the rock pore space with a high level of geometric accuracy at microscale [1].

To experimentally validate and inform the simulation, we have developed a Si/SiO_2 lab-on-chip platform for studying the flow and chemistry of carbon dioxide on well-defined geometries at the microscale. Microfluidic systems have emerged as a tool for studying physical and chemical phenomena at the mesoscale. High-resolution lithography can produce customized microfluidic chips that reproduce the dimensions and geometry encountered in real rock samples and enable studying fluid flow and chemical reactions in environments closer to those in reservoirs. Fabrication of the microfluidic devices follow standard semiconductor process technology, followed by a silicon polishing step and backside through-silicon via etching for fluid delivery into the microchannels from the external pump system. Each separately diced chip is then sealed by anodically bonding a glass cover to allow for optical visualization or spectroscopy. Moreover, to enable studying supercritical CO2 injection conditions, a mechanically resistant flow cell module is being developed to support the chip, provide thermal control and act as the interface to high pressure fluid lines from external pumps.

In this work, we report the progress in the development of microscopy and spectroscopy techniques that can be applied on-chip to monitor the flow of CO_2-laden fluids in constricted geometries. We perform flow experiments on the microfluidic chip and monitor the fluid dynamics in real time using optical microscopy and particle tracing techniques to extract physical properties of the fluid, such as flow speed. This allows to validate the fluid flow in pore network models that provide insight into the percolation of the fluid in real sandstone rock samples. In parallel, we demonstrate how correlative Raman-AFM micro-spectroscopy and other optical microscopy techniques can be employed to estimate rates of CO_2 mineralization and mineral dissolution that will allow us to build and calibrate computational models that consider the joint effects of infiltration and mineralization of CO_2 at the pore scale.

[1] Neumann, R.F., Barsi-Andreeta, M., Lucas-Oliveira, E. et al. High accuracy capillary network representation in digital rock reveals permeability scaling functions. Sci Rep 11, 11370 (2021). https://doi.org/10.1038/s41598-021-90090-0

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