Pore-scale Modelling and Analysis of Reactive Transport in Carbon Storage and Oil Recovery

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In recent years our understanding of reactive transport in porous media has been transformed by X-ray microtomography and NMR imaging. This has had a profound impact in the fields of improved oil recovery, carbon dioxide storage, and groundwater flow. Crucially, pore-scale geometry can now be characterised with ~ 10^9 image voxels, which paves the way to revolutionise the modelling studies of fluid/fluid and fluid/solid reactive transport in heterogeneous rocks. In this PhD project, you will be developing novel modelling methods and analyses for flow, dissolution, and precipitation in Carbon Storage and Improved Oil Recovery. An exemplar study of the impact of initial rock heterogeneity on carbonate dissolution during injection of supercritical CO₂ acidified brine is shown in Figure 1, where dissolved calcite is shown in red in micro-CT images of two carbonates and a beadpack.



Figure 1 Dissolution of (a) Estaillades limestone, (b) Ketton limestone, and (c) beadpack by a CO₂ acidified brine at reservoir conditions. Dissolved regions (shown in red) are most channelized in the most heterogeneous Estaillades limestone (Pereira Nunes et al., 2016).

In this work, a single-component particle tracking method was combined with an elegant streamline-based algorithm to simulate advection, diffusion and reaction. It demonstrated that more heterogeneous rocks undergo more channelized, rather than uniform dissolution, which eventually results in less available surface for reaction and lower reaction rates.

Recently, this work has been considerably expanded by developing a state-of-the-art multicomponent reactive transport simulator (PoreReact) in our group (Oliveira et al., 2018). The simulator can handle complex multicomponent advection, diffusion and reaction in pore space images. An exemplar study on the impact of multicomponent mixing on reversible reaction rates in Portland limestone illustrates well the capability of this approach to examine coupling between transport and reaction in a complex microporous carbonate. Concentration distribution and reaction rates of the products and reactants were observed to be non-uniformly distributed in pore space, in contrast to previous studies on homogeneous media. This behaviour is shown for the main product $CaCO_{3(aq)}$ in Figure 2.



Figure 2 Multicomponent fluid/fluid mixing and reaction in Portland limestone. Two reactant streams injected into the top and bottom half of the image create the main product $CaCO_{3(aq)}$. (a) the product concentration map blue is low and yellow is high) and (b) the product formation rate (blue) and consumption rate (red) (Oliveira et al., 2018).

In this project you will use these two modelling approaches on micro-CT images to visualize and analyse dissolution and precipitation during different injection stages in carbonate rock. Your research will develop novel modelling methodologies based on the experiments to understand coupled transport and reaction behaviour in carbon storage and oil recovery in the subsurface. To this end, you will use High Performance Computing (HPC) facility at Imperial College.

Furthermore, you will have access to experimental X-ray microtomography studies performed at Imperial College, to validate and enhance predictive power of the models. One example is the two-stage dissolution of a composite rock composed of dolomite (bottom half) and calcite (top half) by CO_2 acidified brine, as presented in Figure 3 (Al-khulaifi et al., 2017). Initially, calcite dissolution is uniform, but with a development of a dominant channel in the preceding dolomite, channelized dissolution is observed in calcite.



Figure 3 Visualization of the velocity field at the initial (a), and late stage (b) of injection of CO_2 acidified brine into a dolomite (bottom half) – calcite (top half) composite core. The direction of flow is from the bottom to top. The highest velocities (red) exist at the later dissolution stage, in the single channel spanning through dolomite and calcite (Al-khulaifi et al.,2017).

In this project, the impact of both pore structure and chemical heterogeneity on reaction rates and dissolution/precipitation patterns will be addressed to help design CO_2 and acid injection schemes.

You are invited to join this cutting-edge research project in digital rocks. You will join a world-leading interdisciplinary team in the Department of Earth Science & Engineering at Imperial College London working on all aspects of carbon storage and oil recovery. The successful applicants will be encouraged to publish the research results in internationally recognised peer reviewed journals and present the research results at relevant national and international scientific and professional conferences, and sponsor meetings.

We are looking for students with an outstanding academic record in physical science or engineering including petroleum engineering, applied mathematics, physics, chemistry and chemical engineering. The PhD student will have excellent opportunities to collaborate with academia and industry as part of career development.

This studentship is offered through one of the departmental or university scholarships, including the EPSRC and Imperial College Scholarships. For further details about eligibility criteria, please see information at:

http://www.imperial.ac.uk/earth-science/prosp-students/phd-opportunities/

Please do not hesitate to contact us for further information including informal enquires on:

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References:

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