PORE-SCALE STUDIES OF OCEANIC CO_2 SEQUESTRATION

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The mitigation of CO_2 concentration from the atmosphere while our needs for energy are increasing has attracted significant scientific interest, and various disposal methods (e.g. oceanic, oil reservoirs, saline aquifers, etc.) are under consideration. Direct disposal of liquid CO_2 on the seafloor is one of the approaches for oceanic disposal of CO_2. As its density is higher than that of seawater when the depth is larger than 3000 m, the liquid CO_2 will initially create a pool on the seafloor. In a further step, it will start displacing the seawater in the sediment underneath in a process driven by gravity. At short length scales and/or low infiltration rates (which are expected due to the low permeability of the oceanic sediments), where capillary forces dominate a fingering type displacement is expected, similar to Invasion Percolation (IP) in a destabilizing gradient, since a denser fluid (CO_2) is displacing, downwards, a less dense fluid (water). At large length scales where viscous forces are dominant, a fingering pattern is expected, as well, since we have a less viscous fluid displacing a more viscous fluid.

Additionally, at the CO_2-seawater interface, liquid CO_2 will diffuse into the water and form hydrates with water close to the interface. These processes will modify the porosity and permeability of the seafloor sediment, as well as its composition, affecting thus how deep the liquid CO_2 can penetrate in the sediment. Due to the complex interplay of various phenomena at the micro-level, such processes are difficult to simulate using a continuum hydrogeochemical model.

In this work we have utilized the Lattice Boltzmann (LB) method, a powerful tool in computational fluid dynamics and the Invasion Percolation (IP) in pore networks. These, are two state-of-the-art modeling methods which can be utilized to enhance our understanding of phenomena at the micro-level and enable us to use our findings in refining the macroscopic continuum models.

We have numerically simulated fingering in a two-dimensional channel as well as dissolution and/or precipitation in porous media, two fundamental processes likely to be ubiquitous in oceanic CO_2 disposal. We examined the obtained patterns, as well as the change in porosity/permeability due to hydrate formation and how they depend on various parameters.

Finger penetration in a channel by the LB method

We have studied the effects of viscosity ratio (M), capillary number (u_0), and wettability (θ_1) on finger penetration in a two-dimensional channel using a LB multiphase model. The simulation results show that with an increase of the viscosity ratio or capillary number, both the finger width and the slip distance of the contact lines decrease, while the finger length increases. As shown in Figure 1, with the decrease of the wettability of the displacing fluid, the finger length and its change rate with time increase while the slip distance of the contact lines and its change rate with time decrease, and the minimum capillary number to form a stable finger decreases. Hence, the finger growth is enhanced when the displacing fluid is nonwetting to the wall and otherwise suppressed. An indented part near the beginning of the fingers is clearly observed when a wetting fluid is displacing a nonwetting one. The finger width, however, remains nearly unchanged when the wettability of the fluids changes.

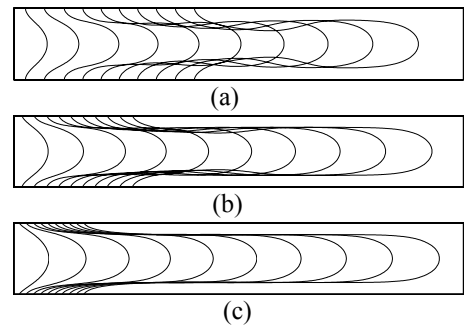

Figure 1: Finger evolution for M=10 at u_0=0.1. (a) θ_1=60°, (b) θ_1=60°, (c) θ_1=119°.

Dissolution and precipitation in porous media by the LB method

We developed a LB model and applied it to simulate fluid flow and dissolution and precipitation in the reactive solid phase in a porous medium. Both convection and diffusion as well as temporal geometrical changes in the pore space are taken into account. The numerical results show that at high Peclet (Pe) and Peclet-Damkohler (PeDa) numbers, a wormhole is formed and permeability increases greatly due to the dissolution process. At low Pe and high PeDa numbers, reactions mainly occur at the inlet boundary, resulting in the face dissolution and the slowest increase of the permeability in the dissolution process. At moderate Pe and PeDa numbers, reactions are generally nonuniform, with more in the upstream and less in the downstream. At very small Pe-Da number, dissolution or precipitation is highly uniform, and these two processes can be approximately reversed by each other. Figure 2 shows the permeability-porosity relationships resulted from these four scenarios.

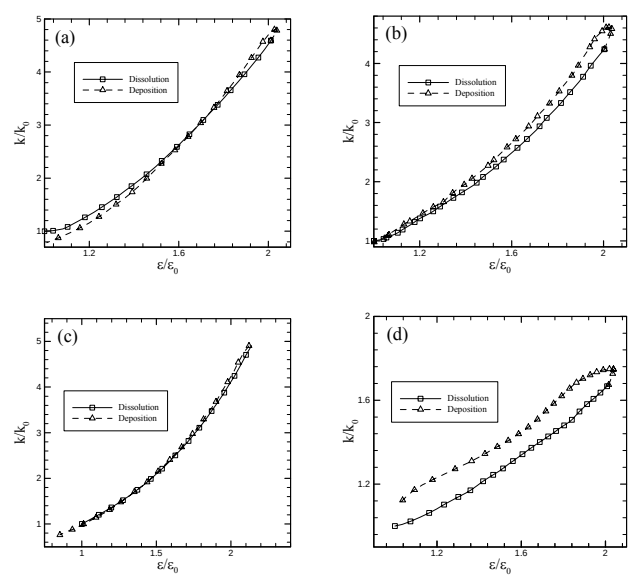

Figure 2: Dependence of permeability on porosity. Both permeability and porosity are normalized by the values of the initial geometry: (a) *Pe*=45, *PeDa*=7.5; (b) *Pe*=0.45, *PeDa*=0.075; (c) *Pe*=0.0045, *PeDa*=0.00075; (d) *Pe*=0.0045, *PeDa*=7.5. Squares denote dissolution and triangles denote deposition.

CO_2 invasion patterns in a pore network

A 2-D pore-network model based on concepts from Invasion Percolation in a gradient was developed to simulate the invasion of liquid CO_2 into the oceanic sediment and the subsequent immiscible displacement of water originally present in the sediment. To capture

the disorder of the oceanic sediment, we assigned random capillary thresholds to the pores during the invasion part of the simulation. This process was also coupled with hydrate formation occurring when the CO_2 entered the Hydrate Stability Zone (HSZ). The reaction process was captured by considering a hydrate forming step, in a pore occupied by CO_2, for every λ invasion steps (smaller λ implies faster kinetics). Figure 3 shows typical invasion patterns obtained for different cases examined, ranging from very fast hydrate formation kinetics (Figure 3a) to essentially no hydrate forming conditions (Figure 3d). Note that at the limit of fast kinetics, as CO_2 enters the HSZ it immediately forms hydrate which results in blocking the pore space, resulting in formation of a thin layer of hydrate which does not allow any further penetration of CO_2 into the HSZ. As a result of the pore blocking, a pool of trapped liquid CO_2 is formed above the HSZ (Figures 3a-b).

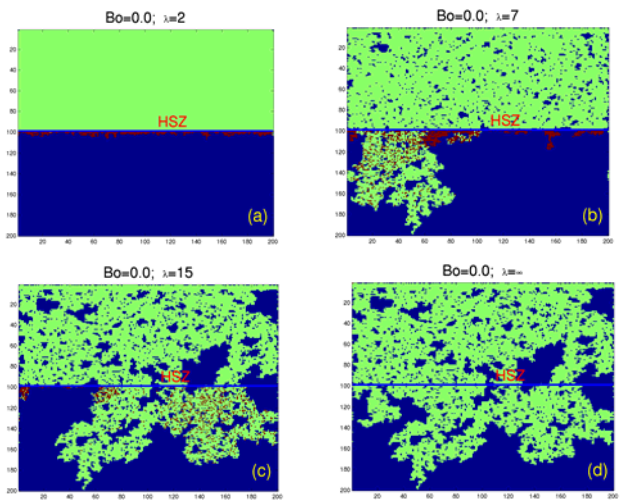

Figure 3: CO_2 invasion patterns in a 200x200 pore-network. Color code: Blue denotes water, green denotes CO_2, and red denotes hydrate.