Numerical and Experimental Investigation of Natural Convection Flow of (Sub-) and (Super-) Critical CO2 in Aqueous Phase

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Abstract

Introduction: Efficient storage of carbon dioxide (CO2) in aquifers requires dissolution in the aqueous phase due to larger available volume for the CO2 to be dissolved in the water initially present in the aquifer and larger partial volume of CO2 in the gas phase. Transfer of CO2 from the gas phase to the aqueous phase would be slow if it were only driven by diffusion. However, dissolution of CO2 in water forms a mixture that is denser than the original water or brine. This causes a local density increase, which induces natural convection currents accelerating the rate of CO2 dissolution [1,2,3]. This study presents a numerical model to simulate a set of high pressure visual experiments, based on the Schlieren technique [3,4], in which we observe the effect of gravity-induced fingers when sub- and super-critical CO2 at in situ pressures and temperatures is brought above a liquid. Use of COMSOL Multiphysics: Numerical modeling of the natural convection model is challenging because high (spatial and temporal) resolution is required in the regions where natural convection takes place. To simulate the instabilities observed in our experiments (see Figure 1), we consider a 2-dimensional cross-section of the cylindrical cell in which the experiments were performed [3]. The diameter of the fluid containing part of the cell is 30 mm and the length 11.6 mm. The cell is approximately filled with water until the equator. For the liquid phase, we use the conventional equations for buoyant density flow, by applying the Boussinesq approximation in 2D, i.e., we take into account the density variation only in Navier-Stokes equation. The boundary conditions are no flow conditions at the vessel boundary. We ignore the boundary conditions for the fluid in contact with the glass windows, assuming that the flow is approximately 2D. For the gaseous phase we only assume diffusion with high diffusion coefficient. Results: The numerical result is illustrated in Figure 2. Conclusion: The main qualitative correspondence between the simulation and the experiment is the existence of a region of high concentration gradient near the gas-liquid interface. However, we observe that in the simulation the onset of instabilities occurs later than the experiments and the wavelengths of the observed fingers are larger in the simulations compared to the experiments. Numerical simulation shows only main fingers that start symmetrically on both sides of the center. This indicates that the simulation of experiments requires a dense grid simulation with much smaller time step sizes.

Reference

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Figures used in the abstract

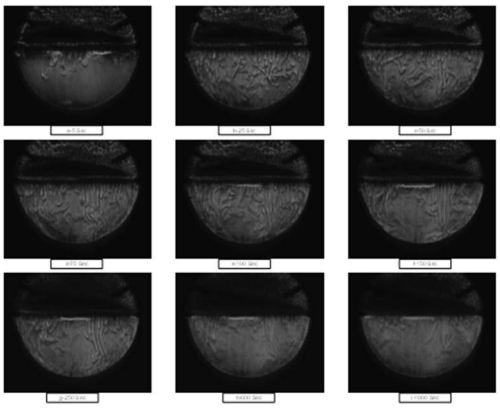

Figure 1: Schlieren pattern in CO2-Water after different times. It shows fingers in the lower half of the circle. The upper half is filled with CO2 at 64 bars and T=312 K.

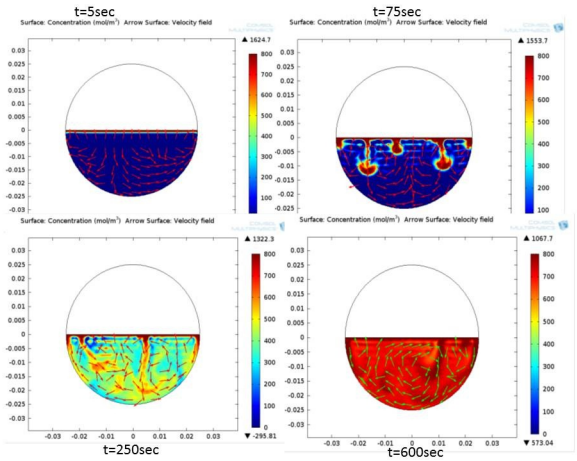

Figure 2: Concentration gradient profiles at t= 5,75,250 and 600 s, p=64 bar and T=312 K.