Parallel simulation of three-dimensional convective mixing in long-term geological CO2 storage in saline aquifers

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Accurate numerical modelling of the effective dissolution rate of aqueous CO_2 solutions is important for analysis of long-term storage efficiency and risk assessments. Theoretical and field studies showed the possibility of switching from a diffusion-controlled mode of dissolution to a natural convection mode which is much more efficient for accelerating the dissolution mechanism. However, most of the previous investigations have been restricted to two-dimensional cross-section models similar to Elder (1947) problem. In this work, we developed a high resolution parallel simulator to investigate these mechanisms with grid blocks needed for accurate modelling of convective mixing in realistic three-dimensional configurations. The simulator sequentially couples groundwater flow and CO_2 transport equations by density and viscosity contrasts. Density and viscosity of the aqueous CO_2 solution is predicted by accurate equations of state module validated against previously published experimental data for a wide range of temperatures and pressures of interest. Numerical experiments show that two-dimensional modelling over-predicts the time to onset natural convection and under-predicts the time to achieve ultimate dissolution of the CO_2-free phase in a homogeneous porous medium. The role of aquifer heterogeneity in further enhancing CO_2 dissolution is illustrated for a generic case study. Heterogeneity leads to a disconnection of the otherwise continuous fingers to form CO_2 blobs and ganglia, increasing the effective surface area between CO_2-rich blobs and formation waters. Results suggest that high resolution three-dimensional modelling should be guided in CO_2 storage projects to (a) estimate the onset of natural convection, (b) determine the size of convective instabilities when they occur, and (c) calculating the maximum mixing achieved.