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Reactive transport modeling of long-term CO_2-brine-rock interactions in heterogeneous deep saline aquifers

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Geological carbon storage (CCS) in deep saline aquifers is a key strategy for mitigating anthropogenic CO_2 emissions due to their widespread occurrence and limited economic use. The long-term fate of injected CO_2 in saline aquifers is controlled by the complex coupling effects of multiphase flow, geochemical reactions, and geological heterogeneity across multiple spatiotemporal scales. However, accurately characterizing and predicting such processes in complex subsurface aquifers remain challenging. As most saline aquifers exhibit inherent geological heterogeneity that may result from primary sedimentary architectures and secondary diagenetic modifications, the roles of multiscale heterogeneity in controlling CO_2 migration and long-term trapping efficiency remain insufficiently understood. Here, we employ high-performance reactive transport modeling using PFLOTRAN on the JURECA supercomputer at Forschungszentrum Jülich to investigate long-term CO_2-brine-rock interactions in heterogeneous saline aquifers that contain multiple sedimentary interlayers with contrasting physical properties that are associated with sedimentary face variations. Geological heterogeneity is established using multipoint geostatistical approaches to reproduce sediemtanry face distributions and hydrological connectivity patterns. Our models integrate multiphase flow, CO_2 dissolution, density-driven convection, aqueous speciation, and kinetically controlled mineral dissolution and precipitation. We systematically examine how spatial heterogeneity in capillary pressure characteristics, porosity, permeability, and initial mineral distributions affect plume migration, solubility trapping, mineral dissolution-precipitation reactions, and the feedback on porosity-permeability evolution. Our results demonstrate that small-scale heterogeneities significantly enhance early-stage CO_2 retention within low-permeability interlayers and channel dissolved CO_2 into finger-shaped flow paths, thereby promoting spatially localized carbonate precipitation. In contrast, more homogeneous models produce a laterally more extensive plume and more uniform CO_2 dissolution patterns and mineral trapping distributions. The dynamic feedback between dissolution-induced porosity enhancement and precipitation-induced clogging gives rise to increasingly complex, self-organized flow-reaction patterns that strongly affect long-term storage efficiency and even storage security. Overall, this study provides new insights into the dynamic interplay between geological heterogeneity and multiphase reactive flow transport processes involved in CO_2 sequestration and contributes to improved geological assessment and performance prediction of CCS in complex subsurface deep saline aquifers.