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Effective models for CO₂ migration and immobilization in large-scale geological systems

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Large-scale models of CO₂ storage in geological formations must capture the relevant geological and geophysical processes that affect the migration and ultimate fate of injected CO₂. These processes span many spatial and temporal scales. For instance, centimeter-scale density-driven convection may enhance CO₂ dissolution across several tens of square kilometers and hundreds of years postinjection. Similarly, recent work has shown that fine-scale topographical variation along the caprock boundary can slow updip CO₂ migration and increase structural trapping over large length and timescales.

Traditional numerical methods cannot solve these large, complex systems over relevant timescales in a practical way because of typical computing constraints. A practical modeling approach is the VE model, which solves coarse-scale vertically integrated governing equations that are coupled with subgrid corrections to capture important small-scale processes, such as local capillarity and convectively driven dissolution, in an efficient and accurate way. The depth-integrated permeability and relative permeability functions that appear in the VE model can also be upscaled to account for structural and topographical heterogeneity at the caprock boundary. The upscaled constitutive equations are derived using a steady-state homogenization approach under the assumption of static capillary equilibrium. This allows the geological system to be simplified for large-scale flow simulations, which can then be more easily coupled with more complex geomechanical or thermodynamical models.