



## Nonlinearity Analysis for Efficient Modelling of Long-Term CO<sub>2</sub> Storage

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Numerical simulation is widely used to predict the long-term fate of the injected CO<sub>2</sub> in a storage formation. Performing large-scale simulations is often limited by the computational speed, where convergence failure of Newton iterations is one of the main bottlenecks. In order to design better numerical schemes and faster nonlinear solvers for modelling long-term CO<sub>2</sub> storage, the nonlinearity in the simulations has to be analysed thoroughly, and the cause of convergence failures has to be identified clearly.

We focus on the transport of CO<sub>2</sub> and water in the presence of viscous, gravity, and heterogeneous capillary forces. We investigate the nonlinearity of the discrete transport equation obtained from finite-volume discretization with single-point phase-based upstream weighting, which is the industry standard. In particular, we study the discretized flux expressed as a function of saturations at the upstream and downstream (with respect to the total velocity) of each gridblock interface. We analyse the locations and complexity of the unit-flux, zero-flux, and inflection lines on the numerical flux. The unit- and zero-flux lines, referred to as kinks, correspond to a change of the flow direction, which often occurs when strong buoyancy and capillarity are present. We observe that these kinks and inflection lines are major sources of nonlinear convergence difficulties.

We find that kinks create more challenges than inflection lines, especially when their locations depend on both the upstream and downstream saturations of the total velocity. When the flow is driven by viscous and gravity forces (e.g., during CO<sub>2</sub> injection), one kink will occur in the numerical flux and its location depends only on the upstream saturation. However, when capillarity is dominant (e.g., during the post-injection period), two kinks will occur and both are functions of the upstream and downstream saturations, causing severe convergence difficulties particularly when heterogeneity is present.

Our analysis of the numerical flux theoretically describes the cause of the convergence failures for simulating long-term CO<sub>2</sub> storage. This understanding provides useful guidance in designing numerical schemes and nonlinear solvers that overcome the convergence bottlenecks. For example, to reduce the nonlinearity introduced by the two kinks in the presence of capillarity, we modify the method of Cances (2009) to discretize the capillary flux. Consequently, only one kink will occur even for coupled viscous, buoyancy, and heterogeneous capillary forces, and the kink depends only on the upstream saturation of the total velocity. An efficient nonlinear solver that is a significant refinement of the works of Jenny et al. (2009) and Wang and Tchelepi (2013) has also been proposed and demonstrated.

### References

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