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Analysis of boundary conditions in numerical simulations of geological CO2 storage

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Simulations of CO2 injection and subsequent migration and reactions can improve our understanding of the long-term fate of the injected CO2 and potentially displaced formation fluids. Particularly, numerical simulations constitute an important tool in the evaluation and planning of geological CO2 storage (GCS) projects, where they can provide an estimates of the storage capacity of given target formations. However, well-defined boundaries for such simulations may be difficult to identify and uncertainty in the nature of the boundaries to deep storage formations typically exists. Furthermore, the choice of boundary conditions potentially has a very strong influence on model predictions, and accordingly, there is an ongoing debate on which boundary conditions (BCs) are most appropriate. Particularly the appropriateness of Dirichlet (open) BCs compared to homogeneous Neumann (closed) BCs has recently been discussed. In this work we perform numerical simulations of CO2 storage in deep saline aquifers surrounded by formations of lower permeability. By including the surrounding media in our simulations we analyze the conditions at the storage formation boundaries. We show that for the case of our study, the appropriate BC is in general neither fully open nor closed, but rather a mixed BC which can be expressed as a relationship between pressure gradient and pressure at the boundary. This type of BC appears to be critical for accurate prediction of the displacement of fluids across the boundary. While it cannot predict fluid displacement, the closed Neumann BC can still reasonably predict the pressure buildup during injection, given that the surrounding medium has lower permeability than the storage formation. The Dirichlet (open) BC is not adequate for this scenario and is also shown to be inadequate for simulation of an infinite storage formation.