# Reactive Transport and Convective Mixing During CO2 Migration in a Saline Aquifer

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## Abstract

Introduction
The capture and storage of CO2 in deep geological formations is one of the proposed solutions to reduce CO2 emissions to the atmosphere. CO2 is injected as a supercritical fluid deep below a confining geological formation that prevents its return to the atmosphere. The solubility of the supercritical CO2 in the resident groundwater (brine) is limited. A configuration of denser CO2-enriched brine overlying lighter water leads to convective flow and the formation of gravity fingers of dense fluid sinking into the resident brine. This process has been acknowledged as an enhancer of supercritical CO2(g) dissolution in saline aquifers (Riaz et al., 2006, Hidalgo et al., 2009, Pau et al., 2010).

However, the CO2-rich brine is not only denser but it has a low pH (around 3.5). Therefore, these fingers can promote chemical reactions if there are carbonated minerals in the aquifer. It is known that geochemical reactions taking place between the CO2, the brine and the rock minerals can affect the permeability and porosity of the geological formation (Luquot and Gouze, 2009). And, on the other hand, these chemical reactions can be enhanced or limited by the changes in the hydraulic parameters. Given the non-linear feedback between reactive transport (dissolution/precipitation), porosity and permeability changes and density driven flow, chemical reactions may affect fingering and convection patterns.

Use of COMSOL Multiphysics®
The interaction between convective mixing and first order chemical reactions has been subject to recent studies (Ennis-King and Paterson, 2007, Ghesmat, 2011, Andres and Cardoso, 2011, Andres and Cardoso 2012). These studies include a first order reaction term in the solute transport equation; however, they don't integrate a fully coupled reactive transport problem. In this work, we use COMSOL Multiphysics® combined with PHREEQC to analyze the interaction between flow and reactive transport processes associated with the dissolution of CO2 in brine in a carbonated aquifer. Fingering of acidic CO2-rich brine can lead to non-uniform calcite dissolution and gypsum precipitation patterns and therefore to heterogeneity in the porosity of the system.

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# Reference

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# Figures used in the abstract

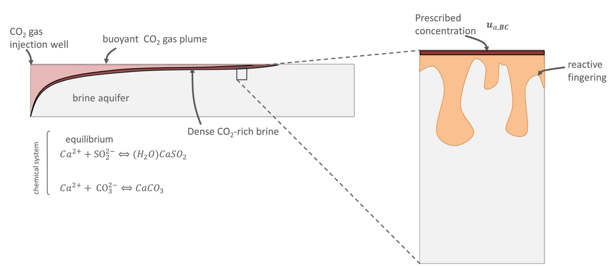


**Figure 1**: Conceptual model of the CO2 cone formed in the aquifer after injection and detail of the density unstable configuration formed that can lead to the formation of fingers of CO2-rich brine.

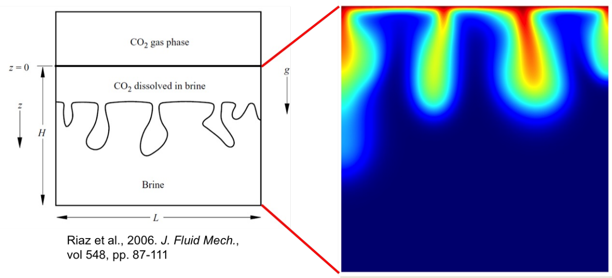


**Figure 2**: Conceptual model (left) and results of the numerical simulation carried out by COMSOL.

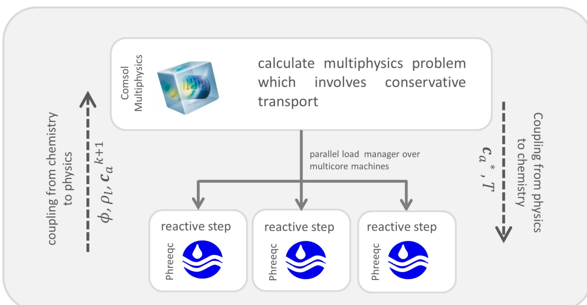


**Figure 3**: Flow chart of the COMSOL-PRHEEQC interface, which combines the key capabilities of PhreeqC and Comsol Multiphysics in a single reactive transport (RT) simulator.

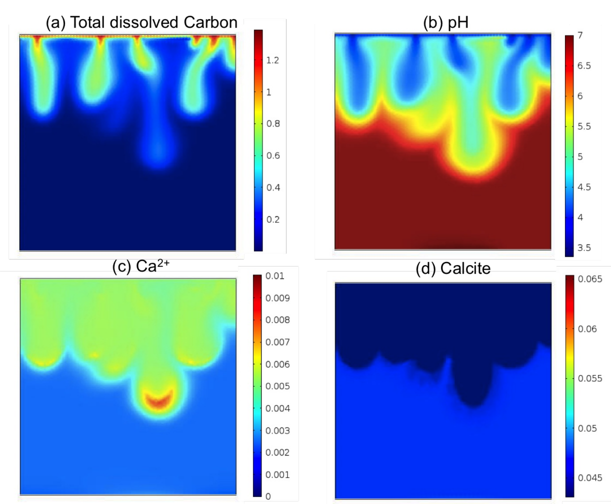


**Figure 4**: Results of the reactive transport problem associated with density driven acidic fingering.