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**A new technique for reactive transport modelling in carbonate reservoirs utilized for CO<sub>2</sub> sequestration**

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Under the Energy Independence and Security Act (EISA) of 2007, the United States (U.S.) Congress authorized the U.S. Geological Survey (USGS) to conduct a national assessment of geologic carbon dioxide (CO<sub>2</sub>) storage resources, which included supporting research to further characterize CO<sub>2</sub> storage resources identified in the assessment. Additionally, the 2007 EISA contains objectives focused on understanding the potential impacts of implementing CO<sub>2</sub> sequestration in subsurface geologic reservoirs. The authors here sought to investigate impacts of CO<sub>2</sub> sequestration in deep saline carbonate reservoirs by incorporating the structural and geochemical complexity and heterogeneity that exists in these systems, and evaluate how that complexity affects physical and chemical processes in the subsurface during CO<sub>2</sub>-plume migration.

Reactive transport modelling is one way of examining the potential impacts of CO<sub>2</sub> sequestration in potential storage reservoirs located within sedimentary basins. Numerous geochemical models simulating injected supercritical CO<sub>2</sub> in saline reservoirs exist; however, much is still to be learned regarding the interaction of supercritical CO<sub>2</sub> with formation waters and mineralogy, specifically in deep saline carbonate reservoirs. Additionally, many current models fail to capture the effects of mineralogical, geochemical, and physical variability typically observed in these reservoirs, and are generally set up with relatively homogeneous systems which do not reflect the true nature of carbonate rock systems. Therefore, a recently created unique tool known as Tough2Cpi is presented here, which models supercritical CO<sub>2</sub> migration and rock-water-CO<sub>2</sub> interactions in porous rock that has mineralogical diversity and intraformational facies changes, in order to improve geochemical and CO<sub>2</sub>-migration predictions in these complex systems. Tough2Cpi is a reactive transport code designed to model the outcome of CO<sub>2</sub> sequestration in structurally and chemically complex reservoirs, and combines the multi-phase, multi-dimensional flow-modelling capabilities of TOUGH2 with The Geochemist's Workbench, a set of software tools for solving a broad span of problems in aqueous geochemistry.

Also presented are the results of a Tough2Cpi simulation that evaluates the potential impacts of CO<sub>2</sub> sequestration in a major deep saline carbonate aquifer of the South Florida Basin, USA that was identified as a potential CO<sub>2</sub> storage resource during the USGS national assessment. This simulation demonstrates the ability of Tough2Cpi to capture the variability in mineralogy and facies distribution throughout the reservoir, as well as the associated spatial variability in porosity and permeability; it incorporates the effects of geochemical, structural, and physical heterogeneity on fluid-rock interactions, and ultimately on modelled CO<sub>2</sub>-plume migration.

