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Numerical Modeling of CO2 Disposal in Saline Aquifers

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The purpose of our research is to develop a systematic, rational, and mechanistic understanding of the coupled processes that would be induced by injection of CO2 into saline aquifers. This is being accomplished by means of conceptual, mathematical, and numerical models that are based on rigorous continuum theories of fluid dynamics, coupled with detailed rock fracture mechanics and chemical speciation and reaction path analyses. Our presentation will review recent progress in process modeling capabilities, and in understanding of the dynamical behavior of CO2 disposal systems.

We have developed a capability for modeling multiphase flows of water and CO2 that includes all possible fluid phase combinations (aqueous - liquid CO2 - gaseous CO2), as well as transitions between supercritical and subcritical conditions. Improvements were made in the accuracy of thermophysical property description, including partitioning of water and CO2 between aqueous and CO2-rich phases, dependence of aqueous phase density on dissolved CO2 content, and treatment of gas mixtures (CO2, H2S, SOx and NOx). These modeling capabilities have been applied to the problem of CO2 leakage from geologic disposal reservoirs along fracture zones and faults, an important objective being to determine whether it is at all possible for CO2 to be discharged in a self-enhancing, eruptive manner. Our simulations provide evidence for strong cooling effects arising from the expansion of supercritical CO2. Eventually sub-critical conditions are reached, where additional cooling may occur when liquid CO2 boils into gas. CO2 discharges may show quasi-periodic cycling due to an interplay between heat transfer and multiphase flow effects.

Strong heat transfer effects were also found in CO2 injection wells, and have been analyzed in connection with a pilot test of CO2 injection that is about to commence in the Frio formation near Houston, Texas. Other studies performed in preparation for this test include modeling of CO2 migration in heterogeneous 3-D media, and design of noble gas tracer tests as a means for characterizing in situ phase conditions.

More fundamental studies have examined hydrodynamic instabilities and the possibility of fingering flow and bypassing as more viscous water is being displaced by less viscous CO2.

Development of a reactive chemical transport code TOUGHREACT has been completed. The code is being released to the public through DOE's Energy Science and Technology Software Center (ESTSC). TOUGHREACT augments our multiphase code TOUGH2 with a comprehensive description of reactions between aqueous, gaseous, and mineral species. Recent applications include CO2 disposal into sand-shale systems as are found in sedimentary formations near the Texas gulf coast, and studies of injection of sour gases that in addition to CO2 contain H2S and SO2.

Geomechanical aspects of CO2 sequestration have been studied using the TOUGH-FLAC simulator that couples TOUGH2 with the commercial rock mechanics code FLAC3D. A newly developed capability for analysis of fault slip and leakage has been tested on a system consisting of a CO2 injection zone that is laterally bounded by two inclined sealing faults. CO2 was injected at high pressure until slip was triggered along the two bounding faults and the amount and the extent of the fault slip were calculated. Material parameters and injection scenarios representing a realistic CO2 injection case were used, similar to those at the Frio test site in Texas. In parallel, the TOUGH-FLAC code is being tested by simulation of in situ experiments, and by code-to-code intercomparison. Additionally, basic studies have been performed to study different fundamental aspects related to underground injection of fluids.