

Simulation of Coupled Processes of Flow, Transport, and Storage of CO₂ in Saline Aquifers

Background

Through its core research and development program administered by the National Energy Technology Laboratory (NETL), the U.S. Department of Energy (DOE) emphasizes monitoring, verification, and accounting (MVA), as well as computer simulation and risk assessment, of possible carbon dioxide (CO₂) leakage at CO₂ geologic storage sites. MVA efforts focus on the development and deployment of technologies that can provide an accurate accounting of stored CO₂, with a high level of confidence that the CO₂ will remain stored underground permanently. Effective application of these MVA technologies will ensure the safety of geologic storage projects with respect to both human health and the environment, and can provide the basis for establishing carbon credit trading markets for geologically storing CO₂. Computer simulation can be used to estimate CO₂ plume and pressure movement within the storage formation as well as aid in determining safe operational parameters; results from computer simulations can be used to refine and update a given site's MVA plan. Risk assessment research focuses on identifying and quantifying potential risks to humans and the environment associated with geologic storage of CO2, and helping to ensure that these risks remain low.

Project Description

This four-year project — performed by the Colorado School of Mines in partnership with Lawrence Berkeley National Laboratory (LBNL) — is developing a comprehensive reservoir simulator for modeling non-isothermal multiphase flow and transport of CO₂ in saline aquifers under varying temperature and pressure conditions. The project focuses on saline aquifers because these formations have the largest potential capacity for CO₂ storage. The simulator models the complex geology of these formations, including heterogeneity, anisotropy, fractures, and faults. The simulator also models geochemical and geomechanical processes that would occur during geologic storage of CO₂. It uses parallel computation methods to allow rapid and efficient modeling assessment of CO injection strategies and long-term prediction of geologic storage system behavior and safety. The experimental plan will expand upon past experience and approaches with multiphase flow experiments at various scales to assess CO, geologic storage. Small-scale test experiments will be used to identify the fundamental processes in homogeneous systems and test the ability of the macroscopic scale models to capture the capillary and dissolution trapping processes in the presence of pore-scale heterogeneities. The model simulations will support the evaluation of geologic storage mechanisms as a viable technique for reducing atmospheric CO₂ emissions.

Goals/Objectives

The primary objective of the DOE's Carbon Storage Program is to develop technologies to safely and permanently store CO₂ and reduce Greenhouse Gas (GHG) emissions without adversely affecting energy use or hindering economic growth. The Programmatic

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PROJECT DURATION

Start Date End Date 10/01/2009 09/30/2013

COST

Total Project Value \$2,000,000

DOE/Non-DOE Share \$1,600,000 / \$400,000

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goals of Carbon Storage research are: (1) estimating CO_2 storage capacity in geologic formations; (2) demonstrating that 99 percent of injected CO_2 remains in the injection zone(s); (3) improving efficiency of storage operations; and (4) developing Best Practices Manuals (BPMs). The primary goal of this project is to develop a state-of-the-art, comprehensive reservoir simulator for quantitative investigations of CO_2 non-isothermal, multiphase flow and long-term storage in saline aquifers. Enhancing this technology will improve estimates of CO_2 storage capacity in geologic formations, better understand CO_2 flow in the subsurface, and demonstrate CO_2 permanence in the subsurface. The simulator will model the complex and coupled physical and chemical processes in CO_2 -brine systems, and will demonstrate:

- Multiphase flow, dissolution, diffusion, and dispersion of CO₂ in the aquifer (Figure 1)
- The effect of temperature on fluid and rock properties, solution and phase behaviors, local heat transfer between fluids and the rock, and global heat transfer both within the aquifer and between the aquifer and surrounding seals
- The effect of geo-chemical processes on long-term dynamics of the aquifer
- · Elevated, pressure-induced rock deformation
- Proper handling of fractures and faults of various scales
- Proper treatment of dissolution-driven instability in the brine phase below horizontally placed CO₂-brine interfaces
- An efficient, robust numerical solution that will be computed implicitly in parallel for rapid assessment of various injection strategies and storage system performance.

Accomplishments

- A rock mechanics module for the reservoir model was modified. The modification includes an expression for how variations in porosity and bulk volume depend on pressure and effective stress.
- A model was set up to study the dissolution of calcite due to CO₂ injection in a one dimensional radial saline formation. After 40 years of injection, the porosity change due to dissolution was found to be less than 0.1% of the original porosity (30%).
- Model simulations have been conducted to study hydromechanical changes during CO₂ injection into a hypothetical aquifer. The model was modified to include thermoporoplastic effects.
- Geochemical reaction modeling is being carried out for the Colorado Plateau, Southern Rocky Mountain, and Gulf Coast sediments. These are formations that have significant CO₂ storage potential.
- A new fully coupled software modification was created to model reservoir flow and rock deformation, and enhancements and improvements were made to the reservoir model to account for mixtures of brine and CO₂, three-phase conditions of gaseous/ liquid CO₂ and water and super- and sub-critical CO₂.

- A new coupled calculation procedure and related algorithm were developed to address the fluid flow, solute transport, and geochemical reaction portions of the model. The updated mathematical equations and solution method were used to solve the fluid flow, solute transport, and geochemical reaction in a simplified isothermal geochemical reaction system. This is the basic principle used to develop the new reactive transport modeling code.
- Simulations of convective mixing with density contrast caused by variable dissolved CO₂ concentration in saline water have been initiated. Additionally, simulations of the In Salah Gas Project were run on a computer cluster to demonstrate the parallel code's ability to simulate larger problems.
- A batch reaction system was used to simulate the reactive geochemistry of CO₂ storage, which includes saline water, CO₂ gas and calcite. Geochemical reactions are fully accounted for and all the chemical reactions involved in this batch reaction system are set to be at equilibrium. The batch reaction model was validated and compared to a commonly used simulator.
- A geochemical reaction module for the reservoir simulator has been developed. This module contains key reactions identified during studies but has been made sufficiently general to allow future extension so that the module can be easily adapted to another saline aquifer with a different set of dominant geochemical reactions.

Benefits

As carbon capture, utilization, and storage (CCUS) capacity increases and projects become commercial beyond 2020, the importance of accurate geologic models and robust risk assessment protocols will become increasingly important to project developers, regulators, and other stakeholders. NETL's Carbon Storage Program aims to continue improvements to the models and risk assessment protocols. Specific goals within the Simulation and Risk Assessment Focus Area that will enable the Carbon Storage Program to meet current programmatic goals are to (1) validate and improve existing simulation codes which will enhance the prediction and accuracy of CO₂ movement in deep geologic formations to within \pm 30 percent accuracy, (2) validate risk assessment process models using results from large-scale storage projects to develop risk assessment profiles for specific projects, and (3) develop basin-scale models to support the management of pressure, CO₂ plume, and saline plume impacts from multiple injections for long-term stewardship in major basins of the United States.

This project research is making significant contributions to the design, modeling, and monitoring of geologic CO₃ storage systems by producing a comprehensive simulator that can fully couple the complex hydro-thermal-mechanicalchemical processes in geologic CO₂ storage. In particular, the proposed development provides a practical approach to evaluate long-term performance of geologic CO, storage systems, and to assess risks associated with a particular system by consideration of fully coupled processes of thermal, geochemical, and rock deformation effects. This research is strategically important to DOE's mission in CO₂ geologic storage and management. Furthermore, once the research goals are achieved, the developed simulator will substantially enhance the ability to predict long-term performance of geologic CO₂ storage systems, from sound engineering design to long-term monitoring.