



High Fidelity Computational Analysis of CO₂ Sorption at Pore Scales in Coal Seams

Background

Fundamental and applied research on carbon capture, utilization and storage (CCUS) technologies is necessary in preparation for future commercial deployment. These technologies offer great potential for mitigating carbon dioxide (CO₂) emissions into the atmosphere without adversely influencing energy use or hindering economic growth.

Deploying these technologies in commercial-scale applications requires a significantly expanded workforce trained in various CCUS technical and non-technical disciplines that are currently under-represented in the United States. Education and training activities are needed to develop a future generation of geologists, scientists, and engineers who possess the skills required for implementing and deploying CCUS technologies.

The U.S. Department of Energy’s (DOE) National Energy Technology Laboratory (NETL), through funding provided by the American Recovery and Reinvestment Act (ARRA) of 2009, manages 43 projects that received more than \$12.7 million in funding. The focus of these projects has been to conduct geologic storage training and support fundamental research projects for graduate and undergraduate students throughout the United States. These projects include such critical topics as simulation and risk assessment; monitoring, verification, and accounting (MVA); geological related analytical tools; methods to interpret geophysical models; well completion and integrity for long-term CO₂ storage; and CO₂ capture.

Project Description

The DOE has partnered with the University of Texas at El-Paso (UTEP) to devise a new mathematical model for understanding CO₂ sorption mechanisms in coal seams. The work by UTEP focuses on devising a new mathematical model utilizing variational techniques for pore size and geometry in order to understand CO₂ transport under multi-phase flow conditions. The project also focuses on techniques to predict the amount of free-phase CO₂ stored in pores due to capillary effects, and describe the interaction between fluid phases and the wide variety of statistical pore shapes that are modeled in the pore network.

The project model is specifically geared for both single- and multi-phase flow in porous media, typical of storage formations for geologic storage of CO₂. First, UTEP is developing a novel computational technique to estimate hydraulic conductance in pore space. Thin section images, micro-CT scanning, simulations of depositional processes, and application of a previously developed hydraulic conductance technique are being performed on a representative sample of a formation type being considered for CO₂ injection. Results from this step are being used to develop a pore network simulation of

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PARTNERS

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PROJECT DURATION

Start Date	End Date
12/01/2009	6/30/2013

COST

Total Project Value
\$288,858

DOE/Non-DOE Share
\$288,858 / \$0



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CO₂ transport (Figure 1), as well as for the trapping and reaction phenomena typical of geologic storage of CO₂. The simulation results are being validated by experimental data provided from a study by Oak Ridge National Laboratory (ORNL). Once the initial pore network simulation is refined, UTEP will develop an iteratively coupled numerical algorithm to solve multiscale phenomena and predict the effects of storage mechanisms and efficiency on a three-phase (water-CO₂-oil) geologic storage system at the reservoir scale. Project research is being conducted primarily by graduate students.

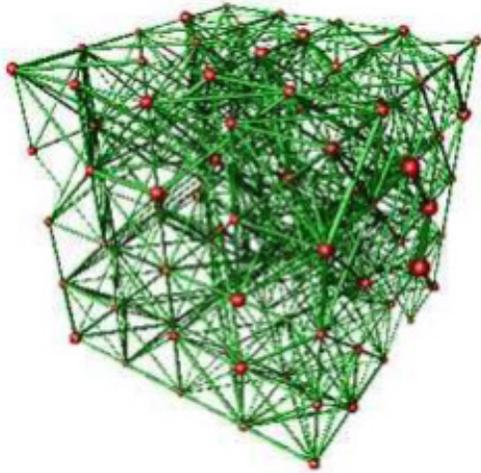


Figure 1: Porescale network model - The microscale model is a discretization of the void space within a porous medium into a network of cylindrical pipes and spherical chambers.

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 goals of Carbon Storage research are: (1) estimating CO₂ storage capacity in geologic formations; (2) demonstrating that 99 percent of injected CO₂ remains in the injection zone(s); (3) improving efficiency of storage operations; and (4) developing Best Practices Manuals (BPMs). The goal of the project is to develop a mathematical pore-network simulation based on coupled variational techniques in order to describe the migration and free-phase trapping kinetics of CO₂ in porous rock in the subsurface, in order to better ensure CO₂ storage permanence in coal seams and other low-porosity geologic materials. In addition, the project provides support for one graduate and one undergraduate student from UTEP to participate in cutting-edge CCUS research. Specific project objectives include:

- Developing a computational technique to estimate hydraulic conductance in pores.
- Constructing and simulating a multiphase system with regular and irregular geometries.
- Improve the fidelity of physics based modeling for better understanding the kinetics of CO₂ trappings inside porous media.

Accomplishments

- As of March 2012, five students had accumulated 4,550 training related hours under the program.
- The project team has developed a high resolution simulator for fluid flow through a porous rock with information obtained from a set of CT-scans taken from a sandstone sample from an oil reservoir. The effort has generated simulations of imbibitions and drainage using simple geometries so that the physics and behavior of the fluid flow could be proven correct.
- A three dimensional computational model has been produced and two-phase Volume of Fluid (VOF) simulations have been performed. A good comparison of the model was obtained using a pore network for the drainage and the contact angle was found to have a significant impact on the micro scale physics in the imbibition simulations. The long term project goal is to simulate fluid flow through real rocks through integrated upscale results from pore-scale to core-scale.

Benefits

The long-term benefit of this project is to advance the fundamental understanding of CO₂ storage capacity and mobility in the presence of oil/natural gas and water/water vapor in geological environments, as well as to quantify interactions within various porous geological materials including coals, shales, and sandstones. Furthermore, the proposed research will create opportunities for preparing outstanding under-represented minority students to join the CCUS workforce as first-class scientists and engineers.

