the ENERGY lab

PROJECT FACTS

Carbon Sequestration

Molecular Simulation of Dissolved Inorganic Carbons for Underground Brine CO_2 Sequestration

Background

Increased attention is being placed on research into technologies that capture and store carbon dioxide (CO_2). Carbon capture and storage (CCS) technologies offer great potential for reducing CO_2 emissions and, in turn, mitigating global climate change without adversely influencing energy use or hindering economic growth.

Deploying these technologies in commercial-scale applications requires a significantly expanded workforce trained in various CCS specialties 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 CCS technologies.

The U.S. Department of Energy's (DOE) National Energy Technology Laboratory (NETL) has selected 43 projects to receive more than $12.7 million in funding, the majority of which is provided by the American Recovery and Reinvestment Act (ARRA) of 2009, to conduct geologic sequestration training and support fundamental research projects for graduate and undergraduate students throughout the United States. These projects will 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 CO_2 storage; and CO_2 capture.

Project Description

NETL is partnering with the California Institute of Technology (CIT) to address the need to measure (in situ) the dissolved inorganic carbon (DIC) in underground brine water at higher sensitivity, lower cost, higher frequency, and over longer periods of time as compared to other MVA efforts for the geologic storage of CO_2. The project will focus on quantifying the risk associated with potential leakage of CO_2 into overlying aquifers. CIT will perform the quantum mechanics (QM) electronic structure calculation on DIC species (e.g., CO_2, bicarbonate ion (HCO_3^-), and carbonate

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PROJECT DURATION

Start Date
12/01/2009

End Date
11/30/2012

COST

Total Project Value
$300,000

DOE/Non-DOE Share
$300,000 / $0

Government funding for this project is provided in whole or in part through the American Recovery and Reinvestment Act.

ion (CO_3^{2-})) to accurately describe the physical sequestration system. QM is a set of scientific principles that describe the known behavior of energy and matter at the atomic and subatomic scale. Electronic structure calculation is a computational approach that can be used to determine the atomic structure of a material and its electronic properties. The QM results will be used to perform a molecular simulation of the DIC species mid-infrared (MIR) spectra at the high-temperatures and pressures representative of sequestration conditions. From this simulation the full MIR spectra will be evaluated using the perturbation theory (a mathematical method to find an approximate solution to a problem that cannot be directly solved) under high-pressure, temperature, and differing pH conditions. The final research simulation results will include the MIR spectra of DIC species and chemistry at real brine conditions (i.e., high salinity, pressure, and temperature).

Goals/Objectives

The project objectives include:

- Providing training to graduate students and professional scientists on molecular simulation of the MIR spectra of the DIC species in water.
- Using molecular simulation to predict the MIR spectra for CO_2 (aqueous) and HCO_3^-, and the changes of the MIR features for DIC species as the pressure, pH, temperature, and salinity change, thus validating and guiding the experimental work that will build the Quantum Cascade Laser (QCL) based spectrometer for underground brine CO_2 sequestration MVA.

Benefits

Overall, the project will make a vital contribution to the scientific, technical, and institutional knowledge base needed to establish frameworks for the development of commercial-scale CCS. Project research will aid in the design of a quantum cascade laser spectrometer that can be used to monitor sequestration sites for possible CO_2 leakage. Through the proposed research, students will be trained with state-of-the-art molecular simulation tools and capabilities that will prepare them to further develop carbon sequestration technologies.