Center for Nanoscale Control of Geologic CO_2

Results of NCGC research are reported in peer-reviewed publications and in our Research Highlights.

The specific overarching goals are to:

(1) establish, within 10 years, novel molecular, nanoscale, and pore-network scale approaches for controlling flow, dissolution, and precipitation in deep subsurface rock formations, to achieve the efficient filling of pore space with injected supercritical CO_2, with maximum solubility, mineral trapping, and near-zero leakage, and

(2) develop a predictive capability for reactive transport of CO_2-rich fluid that is applicable for 100–1000 years into the future.

A collaboration between the SciDAC Applied Partial Differential Equations Center for Enabling Technology (APDEC) and the Energy Frontier Research Center for Nanoscale Control of Geologic CO_2 (NCGC), will extend and further develop the algorithmic and software infrastructure tools, to enable NCGC's goal of modeling molecular-to pore-scale processes in geologic systems.

Center For Nanoscale Control of Geologic CO_2

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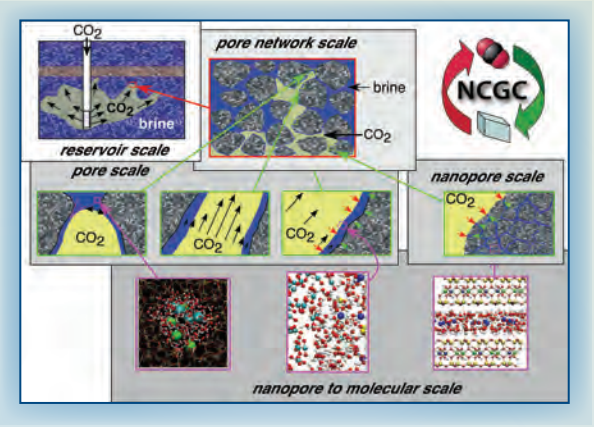
An Energy Frontier Research Center (EFRC)



Collaborative Effort Led By:

Lawrence Livermore National Laboratory
Massachusetts Institute of Technology
Oak Ridge National Laboratory
UC Davis Peter A. Rock Thermochemistry Laboratory
Washington University in St. Louis School of Engineering & Applied Science
The Ohio State University

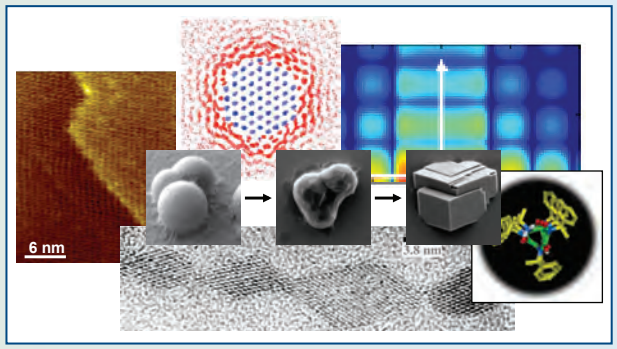
The objective of the Center is to use new investigative tools, combined with experiments and computational methods, to build a next-generation understanding of molecular–to–pore scale processes in fluid-rock systems, and to demonstrate the ability to control critical aspects of flow and transport in porous rock media, in particular as applied to geologic sequestration of CO_2. The objectives address fundamental science challenges related to "far-from-equilibrium" systems, nanoscale processes at interfaces, and emergent phenomena. This DOE Energy Frontier Research Center (EFRC) is a collaborative effort led by Lawrence Berkeley National Laboratory (LBNL), and includes the Lawrence Livermore National Laboratory (LLNL), The Massachusetts Institute of Technology (MIT), the Oak Ridge National Laboratory (ORNL), the University of California campus at Davis (UC Davis) and Washington University in St. Louis. This Center is one of forty-six new U.S. Department of Energy (DOE) Energy Frontier Research Centers (EFRC).

The efforts of the Center investigators are grouped into three Thrust Areas:

- **Controlling Nucleation and Growth**
- **Nanopore Processes**
- **Emergent Processes**

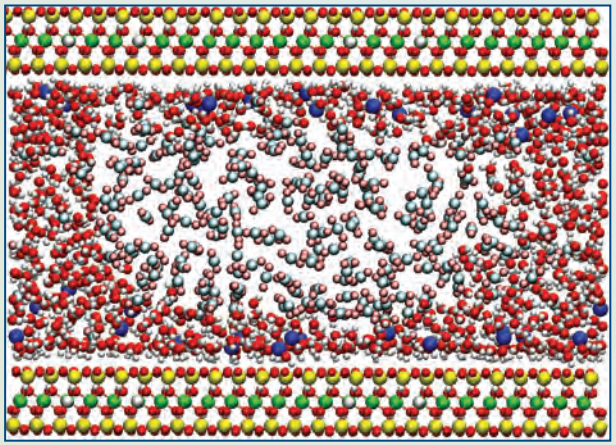
The three Thrust Areas represent groupings of investigators whose work in the Center will be directed at closely allied scientific challenges. However, there are a large number of cross connections within and between these Thrust Areas. The three Thrust Areas have three to six lead scientists, representing all of the institutions involved and constituting the management and scientific leadership of the Center.

Controlling Nucleation and Growth



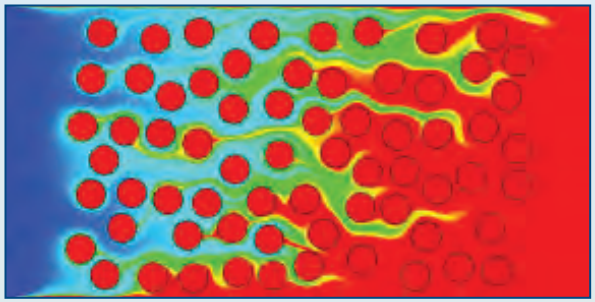
Manipulating the dissolution, nucleation, and growth of minerals in the subsurface requires a detailed understanding of these processes and how they are affected by the special characteristics of porous rock media. The objective of Thrust Area 1 is to develop that understanding at the molecular level, define the role of microbial communities in mediating those processes in reservoir environments, and to explore inorganic, biological and biomimetic methods of directing carbonate mineralization in the subsurface.

Nanopore Processes



One of our major scientific challenges is to understand the behavior of carbon dioxide-rich aqueous solutions confined at high temperature and pressure in nanoporous matrices under geologic sequestration conditions. The goal of research under Thrust Area 2 is to provide a fundamental understanding of these confined carbon dioxide-aqueous solution mixtures, using advanced experimental and computational methodologies to probe fluid behavior from molecular to pore scales.

Emergent Processes



The injection of CO_2 into the subsurface environment drives the fluid-rock system into "far-from-equilibrium" conditions, under which new behavior may emerge that is not predictable by considering processes in isolation. Under these conditions, the strong coupling between flow, transport, and reaction may result in emergent structures and pattern formation that develop within the porous structure of the subsurface at scales ranging from the nano-pore and macro-pore, all the way up to that of a sedimentary basin. These emergent dynamics must be understood in order to predict how CO_2 will behave when injected into the subsurface.