EFRC: CENTER FOR NANOSCALE CONTROLS ON GEOLOGIC CO_2 (NCGC)

UPDATED: AUGUST 2016

AWARDS: $20.0M (August 2009 – July 2014); $12.8M (August 2014 – July 2018)	
WEBSITES: http://science.energy.gov/bes/efrc/centers/ncgc/; http://esd1.lbl.gov/research/facilities/ncgc/	
TEAM: **Lawrence Berkeley National Laboratory (Lead):** Don DePaolo (Director), Jonathan Ajo-Franklin, Benjamin Gilbert, Tim Kneafsey, Peter Schuck, Carl Steefel, Tetsu Tokunaga, David Trebotich, Jiamin Wan; **Oak Ridge National Laboratory**: Larry Anovitz, Gernot Rother, Andrew Stack; **Ohio State University**: David Cole; **Princeton University**: Ian Bourg; **Purdue University**: Laura Pyrak-Nolte; **Stanford University**: Sally Benson, Hamdi Tchelepi; **Washington University, St. Louis**: Young-Shin Jun	

SCIENTIFIC MISSION AND APPROACH

The objectives of NCGC are to provide the fundamental understanding necessary to predict and enhance the performance of underground CO_2 storage systems, and to mitigate problems if they arise during storage operations. Capture and geological sequestration of CO_2 is a potential means of limiting global warming. NCGC uses advanced characterization and modeling tools, combined with specially designed experiments employing purpose-built equipment, to probe the molecular and nanoscale origins of the critical features of fluid-rock systems, with particular reference to CO_2-bearing fluids under carbon storage conditions. The project is organized around three research themes:

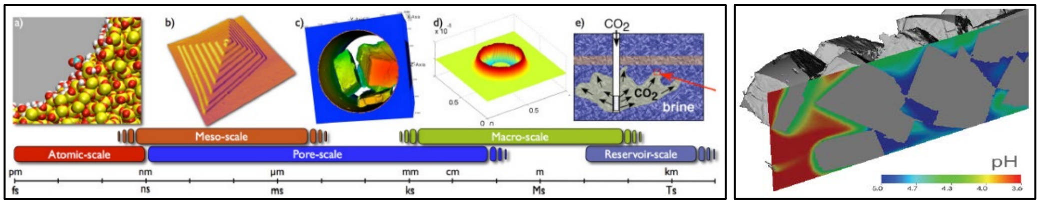
1) **Fractured Shale:** Discover and characterize the key parameters that determine the effectiveness of fractured shales for sealing CO_2 in the subsurface and preventing release back to the surface.

2) **Secondary Trapping:** Quantitatively describe the nanoscale origins, importance and limitations of secondary trapping processes (capillary, dissolution and mineral trapping) for maintaining storage security for long time periods.

3) **Mesoscale Modelling Challenge**: Develop the computational tools and insight necessary to model the mesoscale coupling of nanoscale and molecular processes that determine the material properties and dynamics that ultimately are needed to achieve research themes 1 and 2.

SELECTED SCIENTIFIC ACCOMPLISHMENTS

- Used experiments and modeling to show that shales are robust seals for CO_2, especially when they contain more than 35% clay minerals.
- Determined that organic material and fluid-mineral reactions cause wetting properties to be time-dependent in the subsurface, thus changing the extent of capillary trapping of CO_2.
- Discovered how solution structure and mineral surface templates affect nucleation sites and rates. The studies suggest that preferential nucleation on specific mineral surfaces determines the subsequent porosity and permeability modification in the subsurface.
- Expanded knowledge of supercritical CO_2 ($scCO_2$)-brine-mineral systems with experiments and theory. Measured the thickness of brine films on mineral surfaces in the presence of $scCO_2$, with important implications for the efficiency of capillary trapping.
- Developed an approach for determining mineral reactive surface area that combines 3D X-ray CT, 3D FIB-SEM, and 2D Back-Scattered EM, which was then verified with flow-through experiments.
- Developed an experimental-characterization-modeling workflow that creates digital renditions of subsurface pore structure that became the basis for the largest and highest resolution pore-scale reactive transport simulation of CO_2 injection and trapping ever conducted.
- Used SAXS/SANS to demonstrate interplay between $CaCO_3$ precipitation and nanopore properties.



NCGC research: (left) Carbonate mineral precipitation at various scales. a) Atomic-scale simulation of carbonate adsorption onto a pore wall, b) Single crystal carbonate mineral growth, c) Pore-scale reaction of calcite, d) CO_2 bubble in porous media dissolving host mineral (blue) and precipitating carbonate minerals (red), and e) Illustration of reservoir-scale processes (right) High performance computer simulation results for reactive flow through a $CaCO_3$-filled capillary tube experiment using computational resources at NERSC, with pore scale structure provided by high resolution X-ray synchrotron microtomography carried out at the Advanced Light Source.

IMPACT

- Edited the 2013 and 2015 *Reviews in Mineralogy and Geochemistry (RiMG)* volumes and conducted associated short courses on pore scale geochemical and mineralogical topics.
- Created new specialized experimental systems that can replicate subsurface conditions and allow for *in situ* and *operando* micro-characterization with X-rays and neutrons.
- Developed, with joint DOE SciDAC funding, new high performance computing tools to model pore-scale fluid flow and chemical reactions.
- Ensured industrial relevance by including advisory board members from BP, Exxon-Mobil, and Shell.

PUBLICATIONS AND INTELLECTUAL PROPERTY

As of May 2016, NCGC had published 123 peer-reviewed publications cited over 2,500 times and filed two invention disclosures. The following is a selection of impactful papers:

- Radha, A. *et al.* Transformation and crystallization energetics of synthetic and biogenic amorphous calcium carbonate. *PNAS* **107**, 16438-16443, doi:10.1073/pnas.1009959107 (2010). [**136 citations**]
- DePaolo, D. Surface kinetic model for isotopic and trace element fractionation during precipitation of calcite from aqueous solutions. *Geochimica Et Cosmochimica Acta* **75**, 1039-1056, doi: 10.1016/j.gca.2010.11.020 (2011). [**125 citations**]
- Wallace, A. F. *et al.* Microscopic Evidence for Liquid-Liquid Separation in Supersaturated $CaCO_3$ Solutions. *Science* **341**, 885-889, doi:10.1126/science.1230915 (2013). [**115 citations**]
- Molins, S., Trebotich, D., Steefel, C. & Shen, C. An investigation of the effect of pore scale flow on average geochemical reaction rates using direct numerical simulation. *Water Resources Research* **48**, doi:10.1029/2011WR011404 (2012). [**81 citations**]
- Kim, Y., Wan, J., Kneafsey, T. & Tokunaga, T. Dewetting of Silica Surfaces upon Reactions with Supercritical CO_2 and Brine: Pore-Scale Studies in Micromodels. *Environmental Science & Technology* **46**, 4228-4235, doi:10.1021/es204096w (2012). [**64 citations**]
- Nielsen, M. H., Aloni, S. & De Yoreo, J. J. In situ TEM imaging of $CaCO_3$ nucleation reveals coexistence of direct and indirect pathways. *Science* **345**, 1158-1162, doi:10.1126/science.1254051 (2014). [**86 citations**]
- Cole, D., Chialvo, A., Rother, G., Vlcek, L. & Cummings, P. Supercritical fluid behavior at nanoscale interfaces: Implications for CO_2 sequestration in geologic formations. *Philosophical Magazine* **90**, 2339-2363, doi: 10.1080/14786430903559458 (2010). [**59 citations**]
- Bourg, I. & Sposito, G. Molecular dynamics simulations of the electrical double layer on smectite surfaces contacting concentrated mixed electrolyte ($NaCl$-$CaCl_2$) solutions. *Journal of Colloid and Interface Science* **360**, 701-715, doi:10.1016/j.jcis.2011.04.063 (2011). [**57 citations**]
- Shao, H., Ray, J. & Jun, Y. Dissolution and Precipitation of Clay Minerals under Geologic CO_2 Sequestration Conditions: CO_2-Brine-Phlogopite Interactions. *Environmental Science & Technology* **44**, 5999-6005, doi:10.1021/es1010169 (2010). [**51 citations**]