Center for Nano-scale Controls on Geologic CO_2
New Insights on CO_2 Trapping

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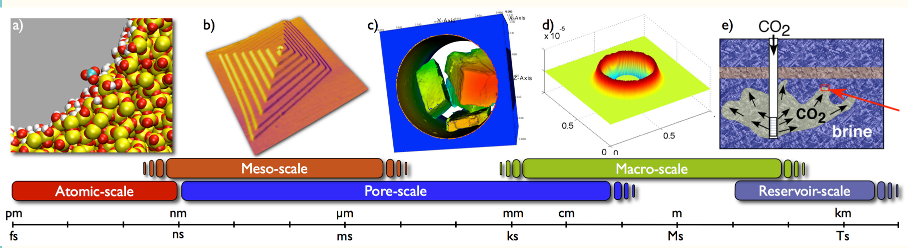
MISSION

To enhance the performance and predictability of subsurface storage systems by understanding the molecular and nanoscale origins of CO_2 trapping processes, and developing computational tools to translate to larger-scale systems



TECHNICAL OVERVIEW

The vision for the Center is to understand, predict, and enhance the performance of underground CO_2 storage systems. Specific 4-year goals are to produce (1) a next-generation understanding of the nanoscale-to-mesoscale chemical- mechanical behavior of shale - a critical material for a low-carbon energy future, (2) quantitative models for the efficiency of reservoir capillary trapping and its effect on solution and mineral trapping, (3) methods to predict mineralogical trapping, and (4) theory, experimental data, and computational tools to allow nanoscale effects to be translated to mesoscale and continuum scale model equations and parameters.

RESEARCH OBJECTIVES

Scientific gaps the Center is addressing:

- The origin and evolution of wetting properties of complex, reactive fluids in contact with common minerals encountered in carbon storage
- Reactivity between fluids and minerals in nanoporous to macroporous rocks
- Long term-evolution of capillary-trapped CO2
- The response of fractured shale to intrusion of CO2-containing mixed fluids
- Theory and computational tools that allow the large scale and long-timescale evolution of fluid-rock systems to be simulated such that they reflect the nanoscale and mesoscale properties of geological materials at far-from equilibrium conditions.

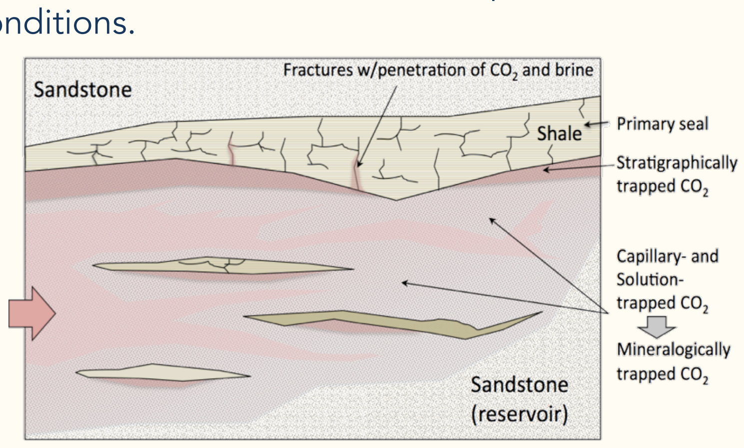


Figure 1: Schematic illustration of key short- and longer term trapping processes that must operate to ensure quantitative storage of injected CO_2 for >1000 years (Benson and Cook, 2005).

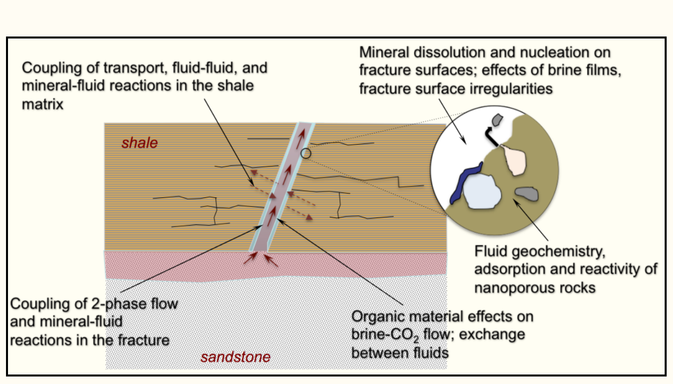


Figure 2: Processes and issues relating to the evolution of fractures in shale.

ACKNOWLEDGMENTS

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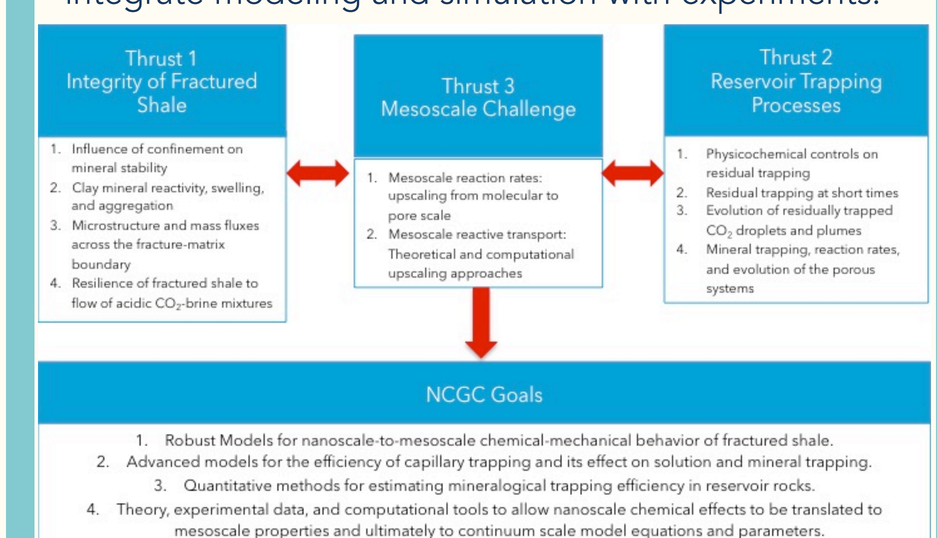
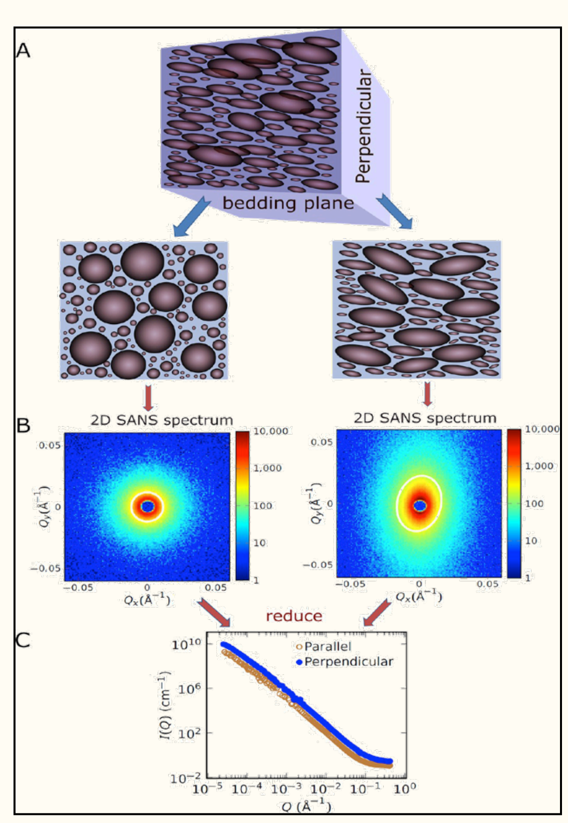
RESEARCH AREAS

The research of the NCGC is divided into three Thrust Areas that address (1) the sealing effectiveness of fractured shales, (2) reservoir processes that control secondary trapping (capillary, dissolution and mineral trapping) and (3) developing the computational tools and insight necessary to model mesoscale couplings and material properties and dynamics. Systems of study include well-characterized natural rock and mineral samples, and synthetic materials fabricated by established methods and methods to be developed. A key aspect of our approach is to bring multiple characterization methods, and diverse complementary expertise, to bear on the same experiments, and to integrate modeling and simulation with experiments.

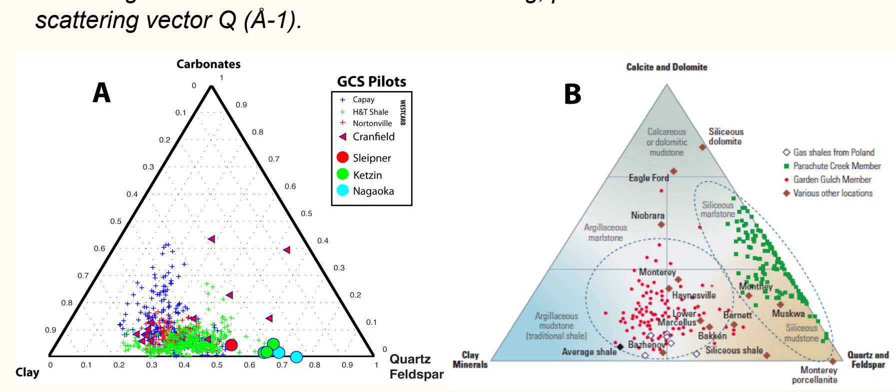


STRATIGRAPHIC TRAPPING BY FRACTURED SHALE – THRUST AREA 1

Thrust Area 1 aims to provide an understanding of the nanometer to meter scale properties of seal rocks and fractures. The research plan is structured around four phenomena: the geochemistry of confined fluids, mineral reactivity and colloid generation at fracture surfaces, coupled mass transfer and mineral reactivity at the boundary between the fracture and the rock matrix, and coupled multiphase flow, geochemistry, and geomechanics in the fracture itself.



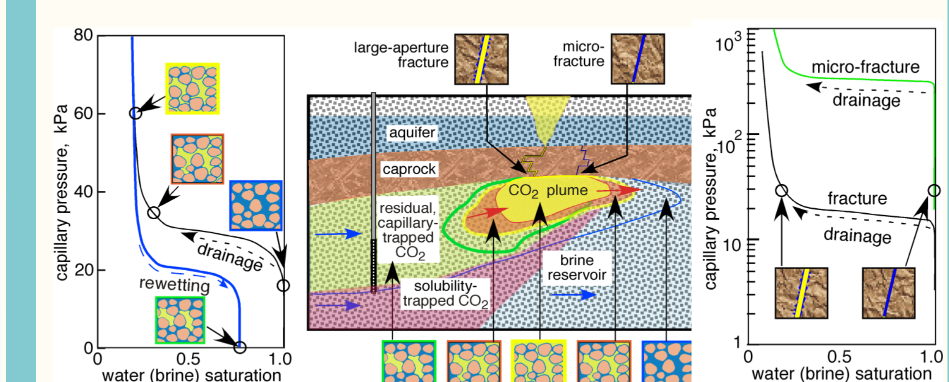
(A) Grains shapes in shale cut // or ⊥ to the bedding. (B) 2D SANS spectra for sample cut //(left) and ⊥ (right) to bedding; (C) SANS and USANS neutron scattering intensities cut // and ⊥ to the bedding, plotted as functions of the scattering vector Q (Å-1).



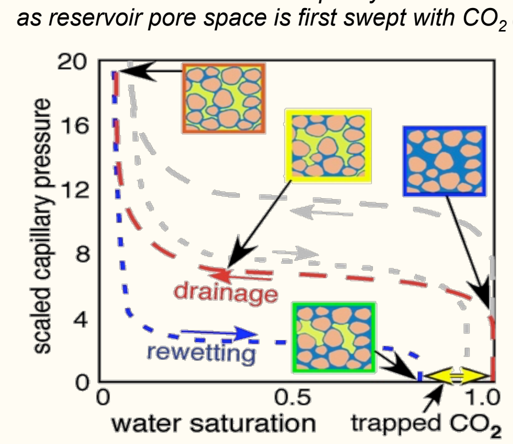
Three-component diagrams illustrating the main mineralogical variations in shales that constitute carbon storage seals at several past and current GCS sites (A) as well as hydraulic fracturing targets (B) for natural gas production (Allix et al., 2011).

RESERVOIR TRAPPING PROCESSES– THRUST AREA 2

Thrust Area 2 aims to provide a better understanding of storage security beyond the stratigraphic seal; to quantify the residual and mineral trapping of CO2 in GCS reservoirs. The research plan is structured around 4 tasks, investigating physicochemical controls on residual trapping, residual trapping estimates at short times, the long term stability of residual storage, and mineral trapping processes.



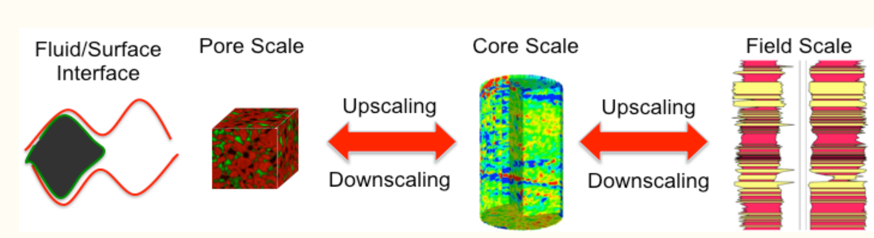
Schematic of the effect of capillary forces on the distribution of brine and $scCO_2$ as reservoir pore space is first swept with CO_2 ("drainage") and then re-wetted.



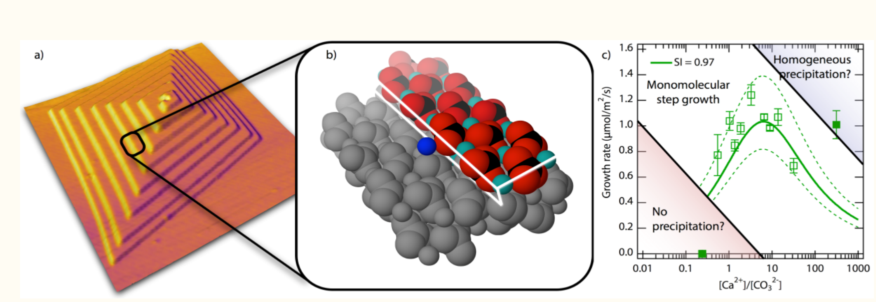
Drainage and imbibition capillary pressures (red and blue curves, respectively) for $scCO_2$-brine in limestone sand are much lower than expected based on pore sizes and interfacial tensions (gray dashed and dotted curves, respectively). Trapped CO_2 fractions are higher than predicted.

MODELING APPROACHES FOR THE MESOSCALE CHALLENGE– THRUST AREA 3

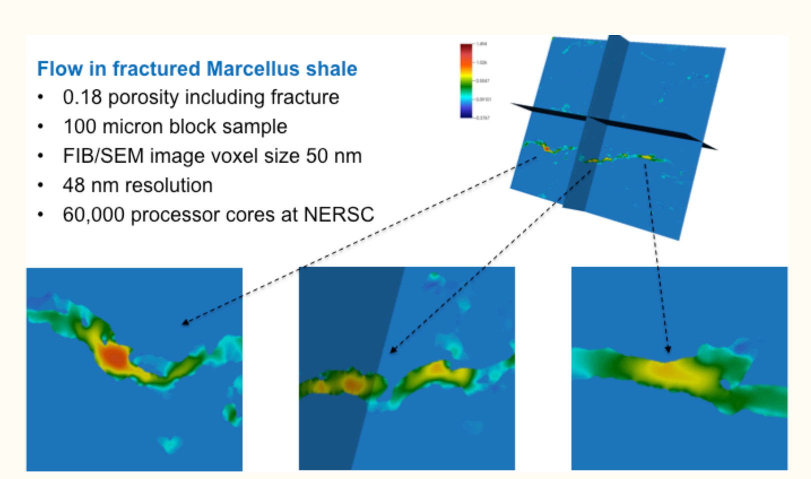
Thrust Area 3 aims to build on the progress made in NCGC to address the mesoscale challenge from the DOE BES Basic Research Needs report From Quanta to the Continuum: Opportunities for Mesoscale Science. This Thrust is organized into three topics on 1) Mesoscale Reaction Rates: Upscaling Reaction Rates from Molecular to Pore Scale, 2) Mesoscale Fractures: Modeling Fracture Networks, and 3) Mesoscale Reactive Transport: Theoretical and Computational Approaches for Upscaling to the Mesoscale.



Hierarchy of scales relevant for multiphase flow, transport, and reaction modeling that will be linked as part of the proposed research.



Process-based models.



NCGC can now fully resolve flow in fractured shale and other subsurface materials.