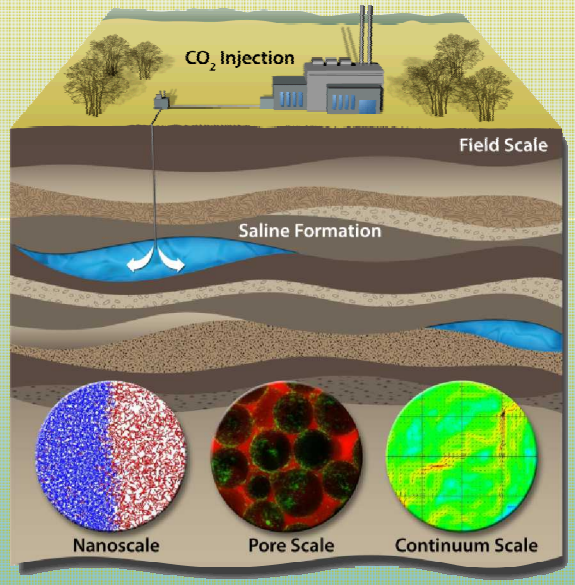
SAND2013-4021C

Center for Frontiers of Subsurface Energy Security



Marianne Walck, Gary A. Pope, Susan Altman, and Mojdeh Delshad

The 12th Annual Carbon Capture Utilization & Sequestration Conference
Pittsburgh, Pennsylvania
May 15, 2013

Sandia National Laboratories

U.S. DEPARTMENT OF ENERGY
Office of Science

TEXAS

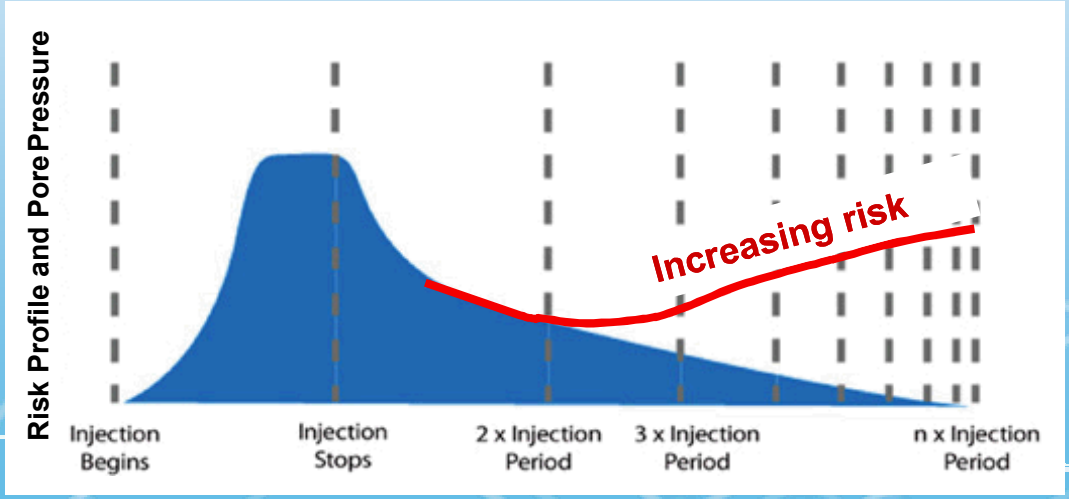
Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

NNSA

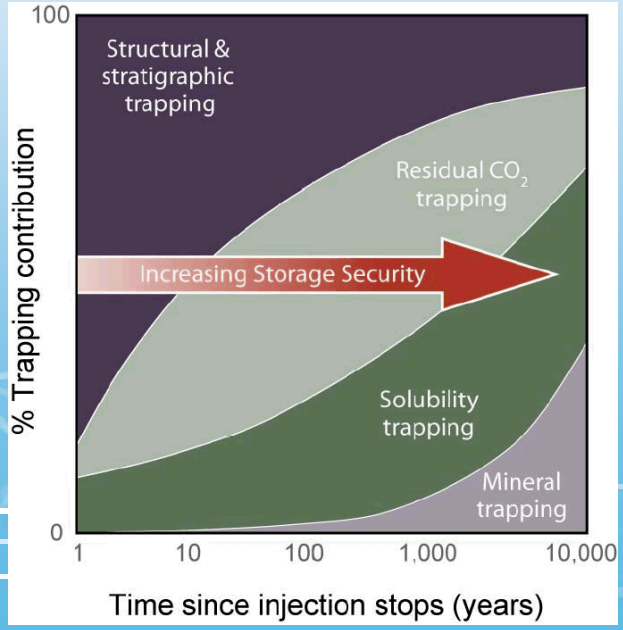
Science to Inform Geological CO_2 Storage Security

Basic Science → Risk Assessment → Mitigation and Management

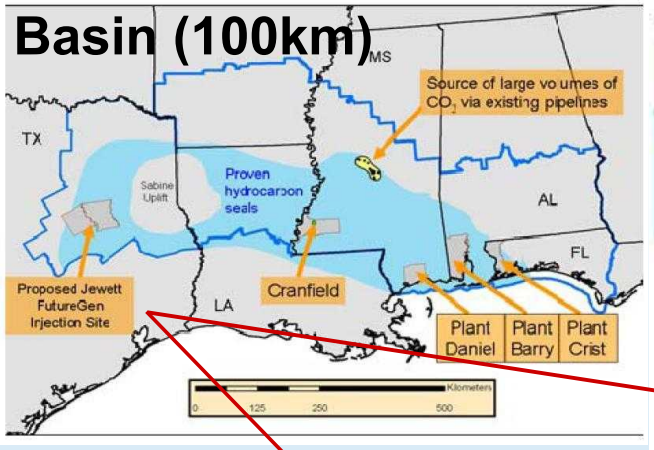
- **GOAL 1: Develop, improve, and test multiscale models for multiphase, multicomponent, multiphysics phenomena during CO_2 injection and migration.**
- **GOAL 2: Use observations at field sites and experimental data to inform models.**
- **GOAL 3: Develop models and methods for improved prediction of large-scale and long-term behavior of stored CO_2.**

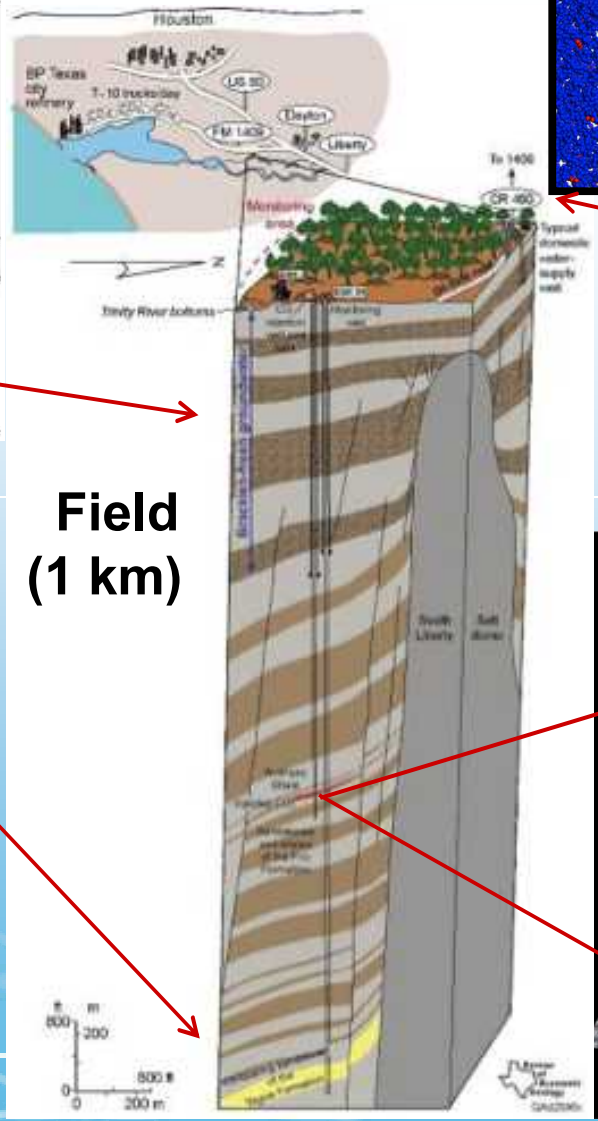


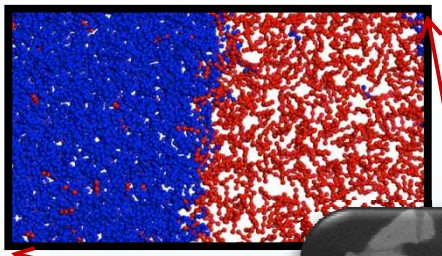
Benson, IPCC, 2007



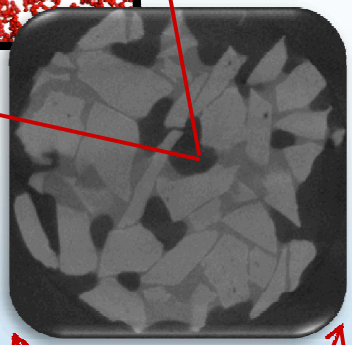
Spanning Scales Range from Molecular to the Field and Femtoseconds to Millennia



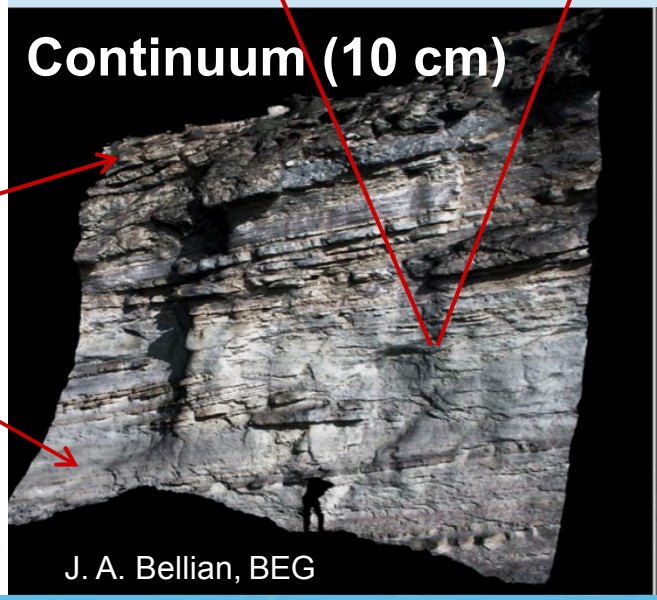




Molecular
(1 nm)



Pore
(10 μm)



Geosystems are large and highly heterogeneous.

Five Accomplishments

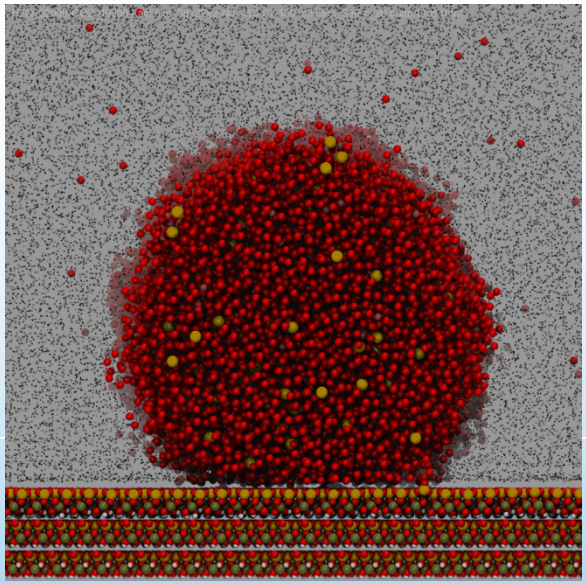
- Pioneering work in molecular dynamics coupled with experiments have implications for the science of CO_2-mediated geochemistry
- Established synergistic experimental and modeling capability for the science of fluid-driven geomechanics
- Provided a new understanding of the evolution of CO_2 leakage pathways
- Provided first field-based assessment of the relevance of solubility trapping for storage security
- Created seismic inversion technique opening new possibilities for crustal observation

Pioneering Molecular Dynamics

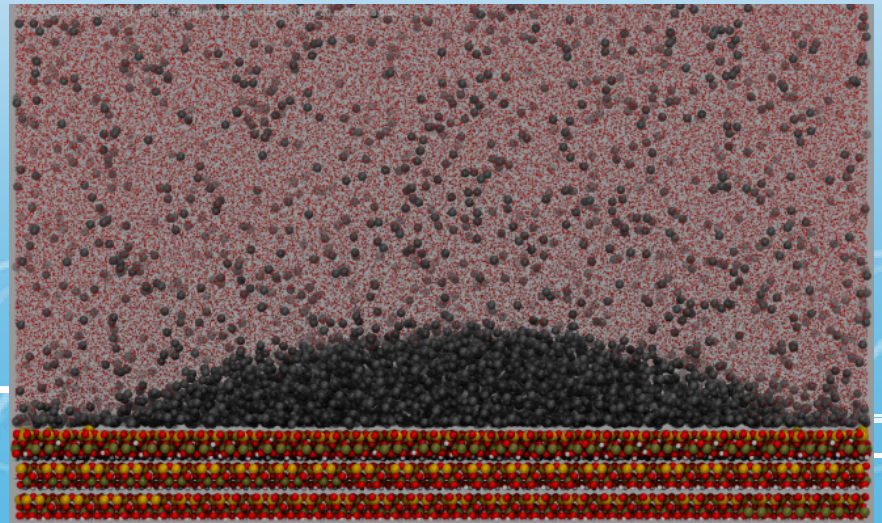
Hydrophobic

kaolinite (siloxane-like) surface

0.7M NaCl in CO_2



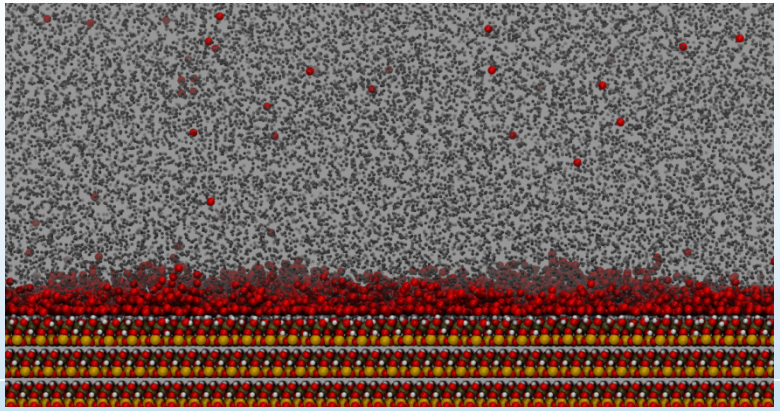
CO_2 in H_2O



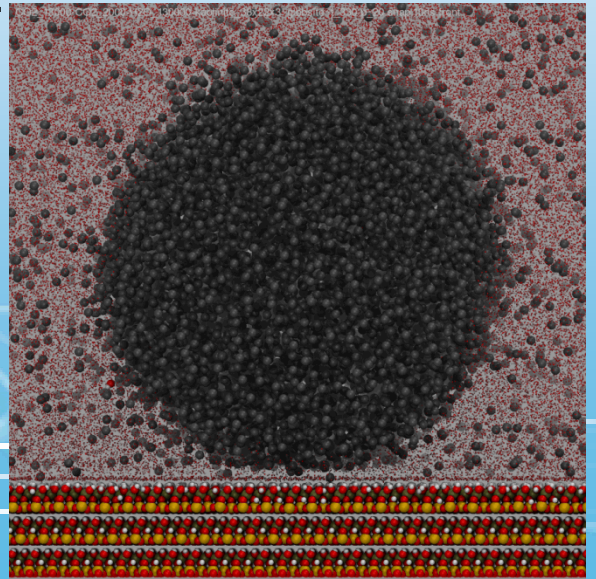
Hydrophilic

kaolinite (gibbsite-like) surface

H_2O in CO_2



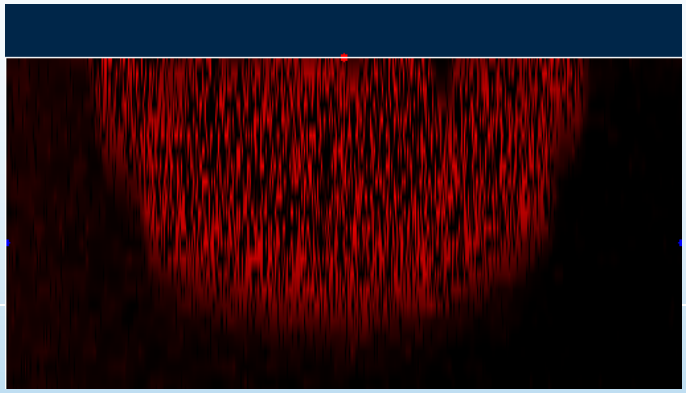
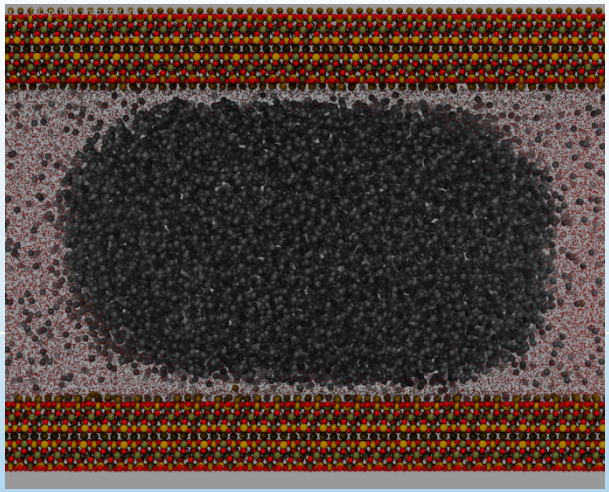
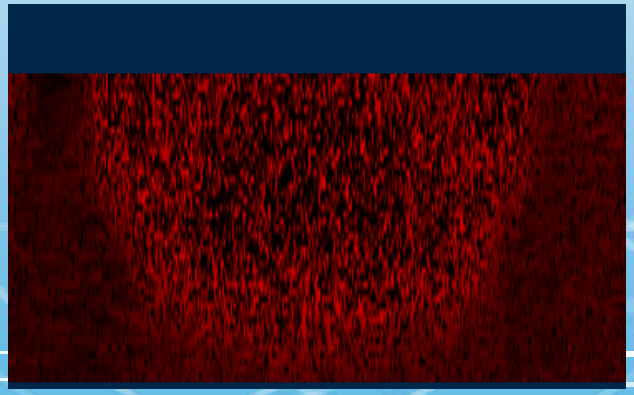
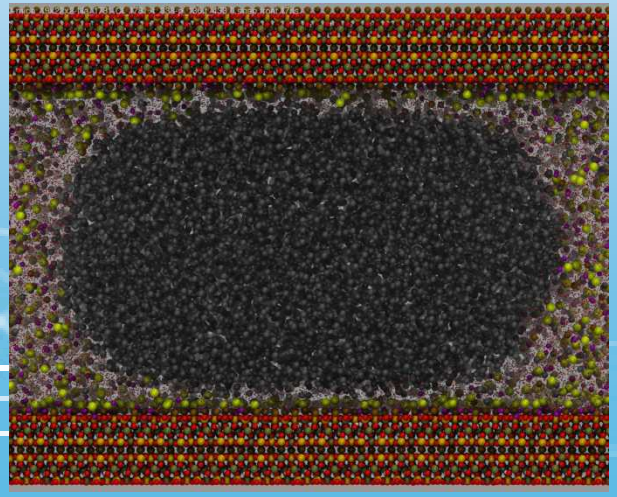
CO_2 in H_2O



Cygan, Romanov, and Myshaki, *Journal of Physical Chemistry C*, 2012.

Pioneering Molecular Dynamics

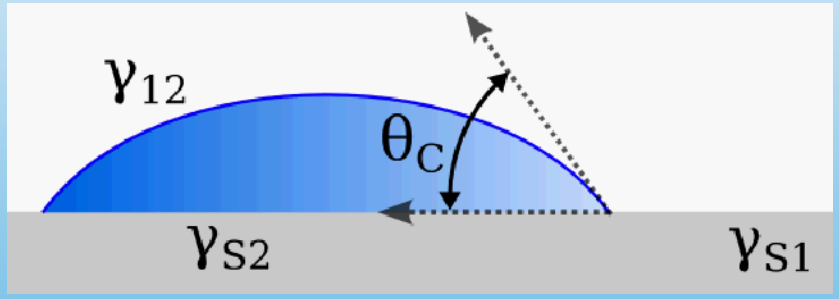
CO_2 contact angles on clean muscovite surfaces

	confocal microscopy of sessile micro-droplets	simulation of droplets in 10 nm slit pores
CO_2 in H_2O		
CO_2 in 1.7M NaCl		

Pioneering Molecular Dynamics

Linking the sub-pore-scale to the pore- and field-scales

- interfacial tension γ_{12}
  - surface free energy
- contact angle θ_C
  - indication of wettability



$$\gamma_{S1} - \gamma_{S2} = \gamma_{12} \cos\theta_C$$

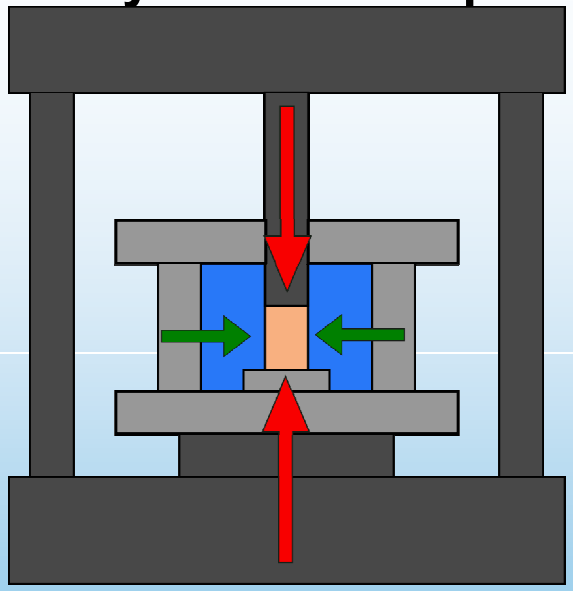
- capillary pressure p_c
  - overpressure required to displace current fluid with new fluid

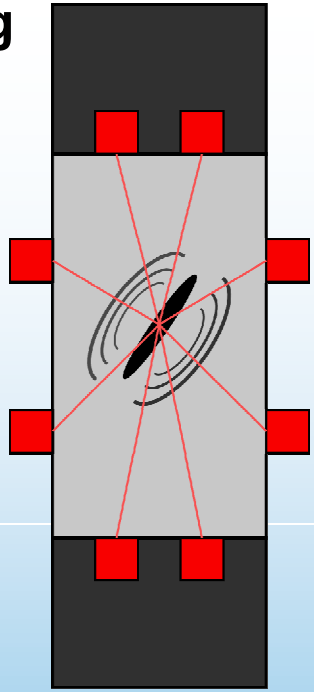
$$p_c = \frac{2\gamma_{12}\cos\theta_C}{r}$$

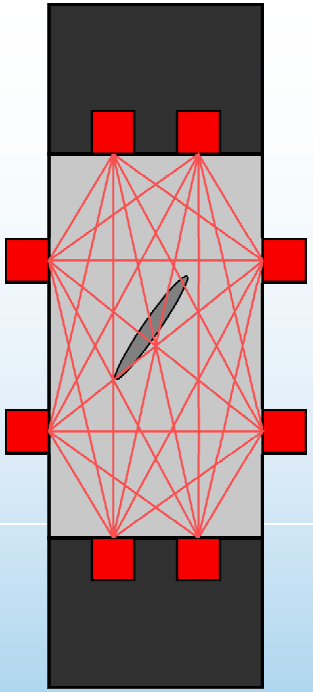
- relative permeability
  - fractional permeability of a fluid in the presence of other fluid(s)

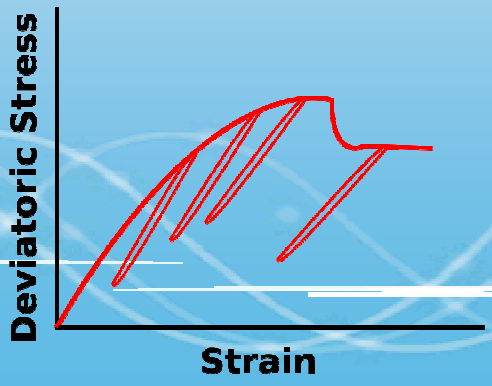
Fluid Driven Geomechanics

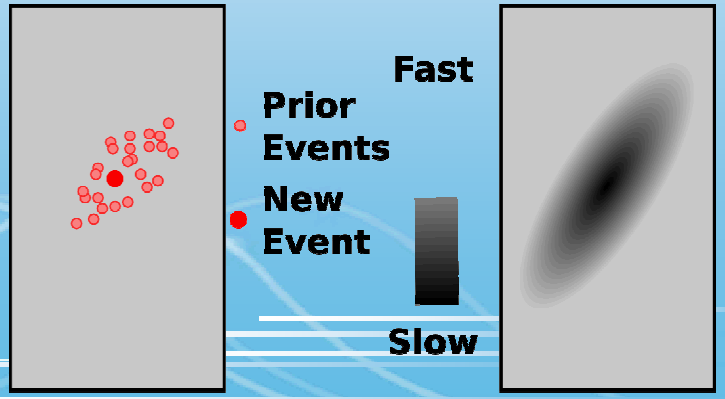
Developed a new technique for measuring dynamic, static, and elastic moduli simultaneously for shale caprocks





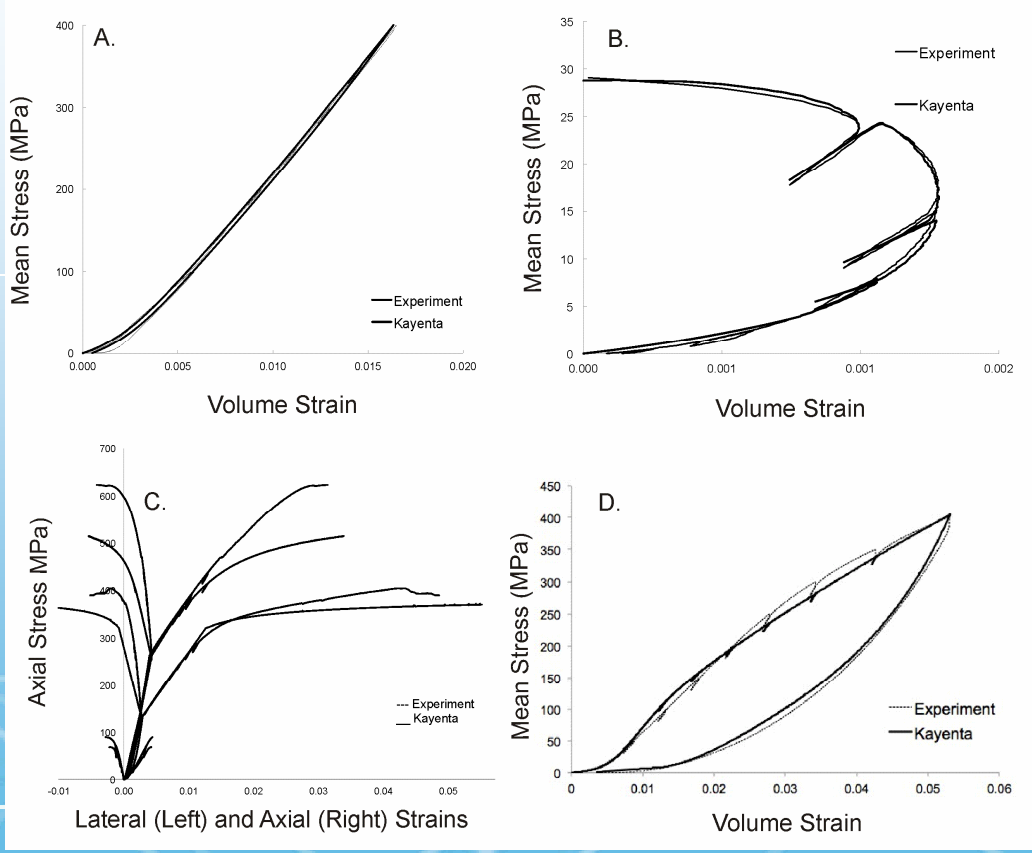






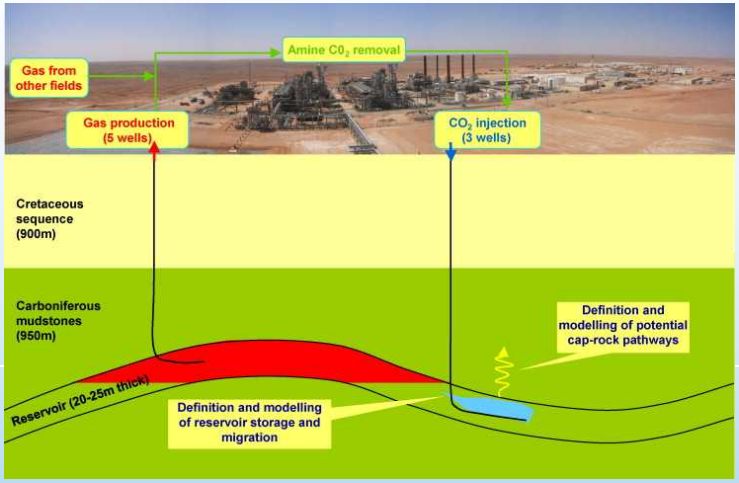
Fluid Driven Geomechanics

Validated a constitutive model for elastic-plastic deformation of saline formation sandstone reservoirs

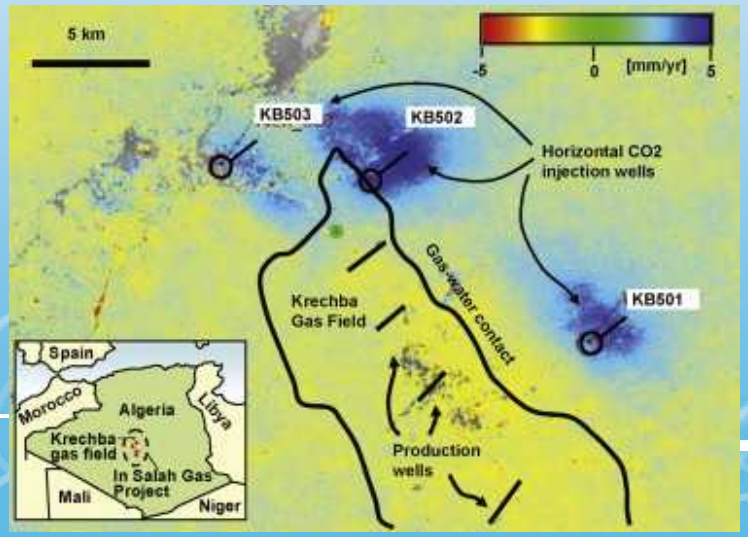


Fluid Driven Geomechanics

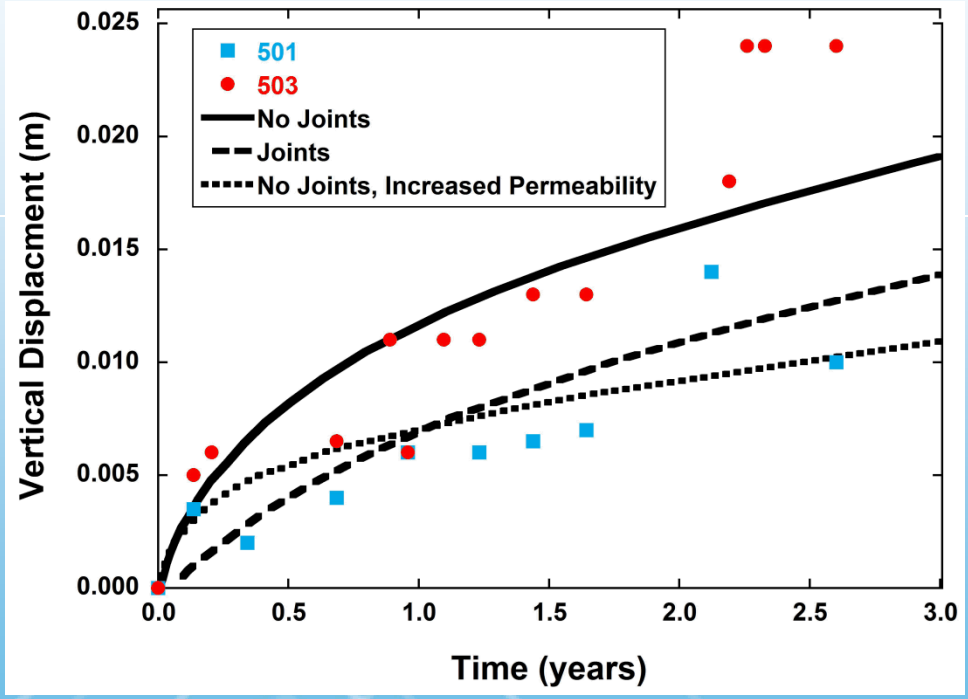
Including joints in the geomechanical constitutive model allows prediction of observed surface uplift at the In Salah storage site.



Iding et al. 2010



(Rutqvist, 2012)



Evolution of CO_2 Leakage Pathways

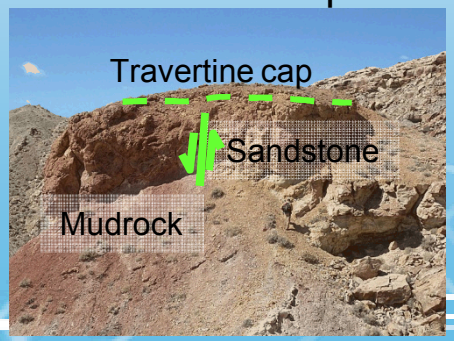
Whether faults act as conduits or barriers in the context of CO_2 storage is an emergent phenomenon

Natural CO_2 leakage at Little Grand Wash Fault, Utah (Crystal Geyser)

Small-scaled coupled flow and geochemistry responsible for large-scale migration patterns

Escaping CO_2 tends to seal its escape path

Fossil Seep



Active Seep

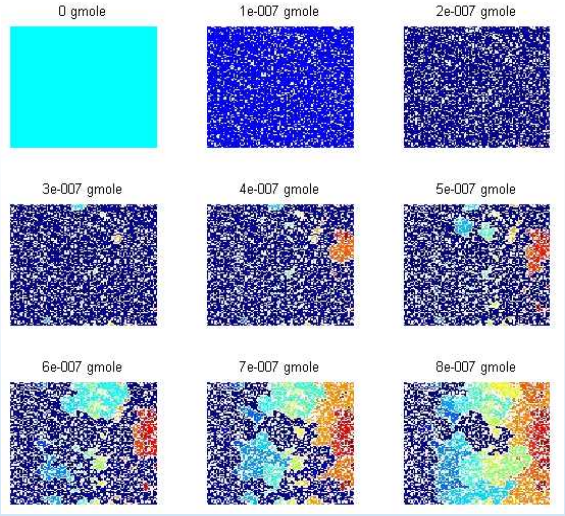
~ 25m

~ 0.8m

Evolution of CO_2 Leakage Pathways

Modeling Predictions:

Multiscale modeling predicts permeability reduction at the continuum scale



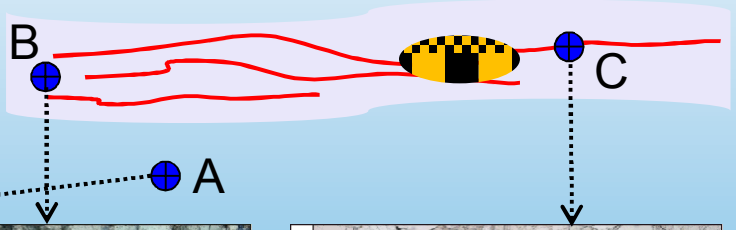
Field Observations:

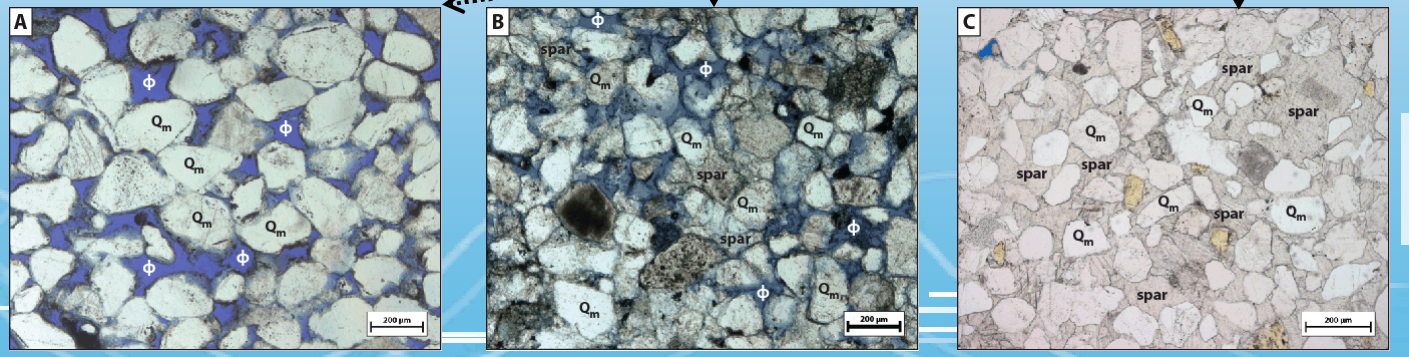
Increasing pore-filling within the fault zone → decreasing permeability → lateral migration of the fault

Implications:

Small-scaled coupled flow and geochemistry responsible for large-scale migration patterns

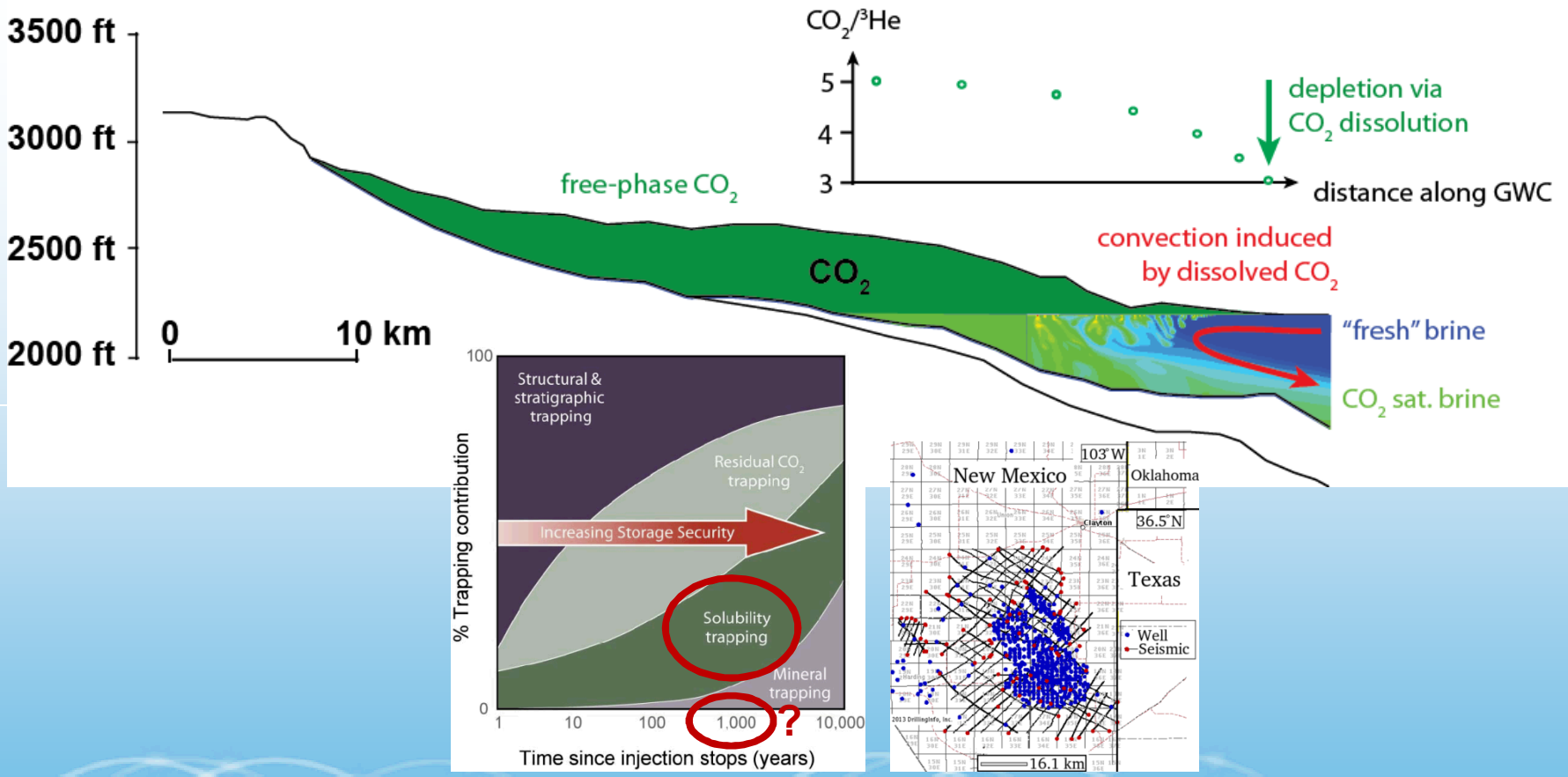
Escaping CO_2 tends to seal its escape path





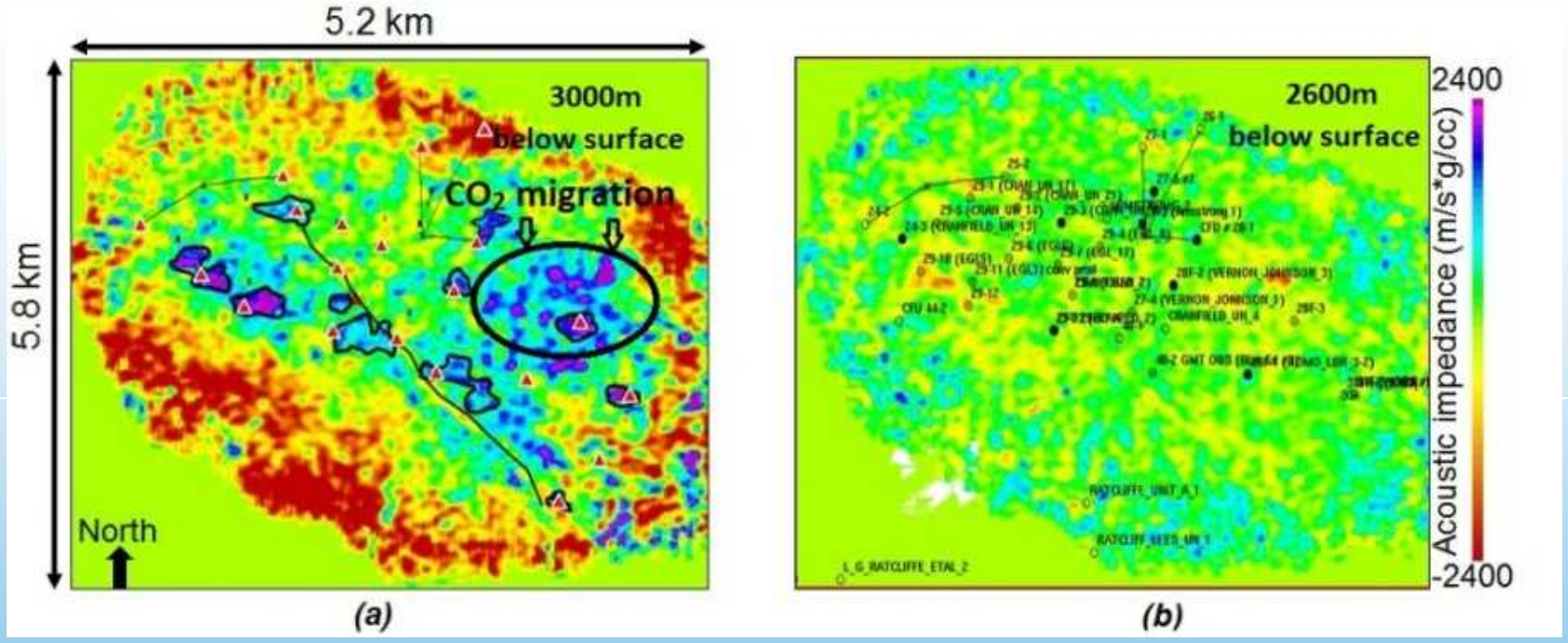
Increasing amounts of pore-filling material

Field-Based Assessment of Solubility Trapping



Magmatic CO_2 injected approximately 10,000 years ago.
Why is the CO_2 still there?
What is the rate of CO_2 dissolution?

Innovative Seismic Inversion Technique



Injected CO_2 migrated mostly along the top layer of the storage reservoir for the Cranfield CO_2 injection demonstration

Evidence of leakage through the reservoir seals is not observed

Zhang, Sen, Phan and Srinivasan, Journal of Geophysics and Engineering, 2012
Zhang, Ghosh, Sen, and Srinivasan, International Journal of Greenhouse Gas Control, In Press

Five Accomplishments

- Pioneering work in molecular dynamics coupled with experiments have implications for the science of CO_2-mediated geochemistry
- Established synergistic experimental and modeling capability for the science of fluid-driven geomechanics
- Provided a new understanding of the evolution of CO_2 leakage pathways
- Provided first field-based assessment of the relevance of solubility trapping for storage security
- Created seismic inversion technique opening new possibilities for crustal observation