*Exceptional service in the national interest*

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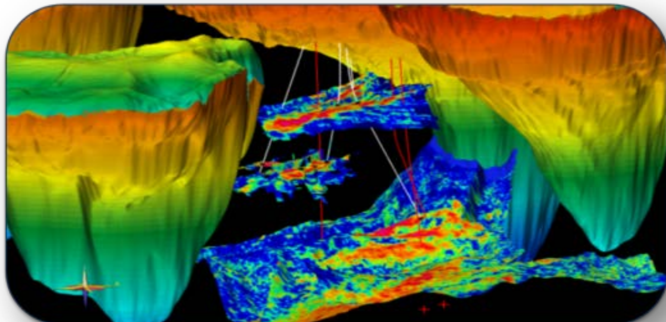

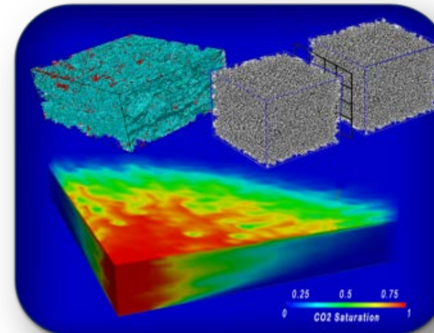


# The Science of $CO_2$ Management:

## The Center for Frontiers of Subsurface Energy Security (CFSES), a DOE Energy Frontier Research Center (EFRC)

**Marianne C. Walck, Ph. D.**

Sandia National Laboratories, Vice President of California Laboratory and Energy and Climate Program Management Unit

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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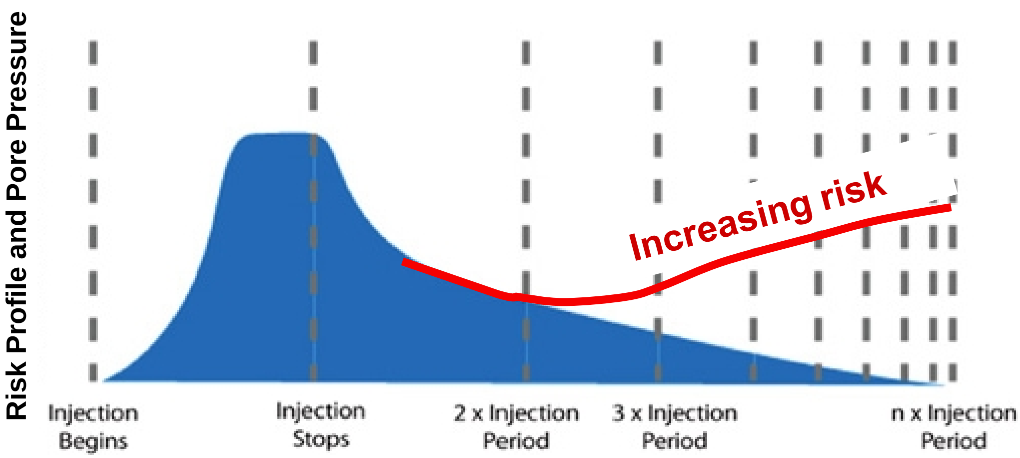
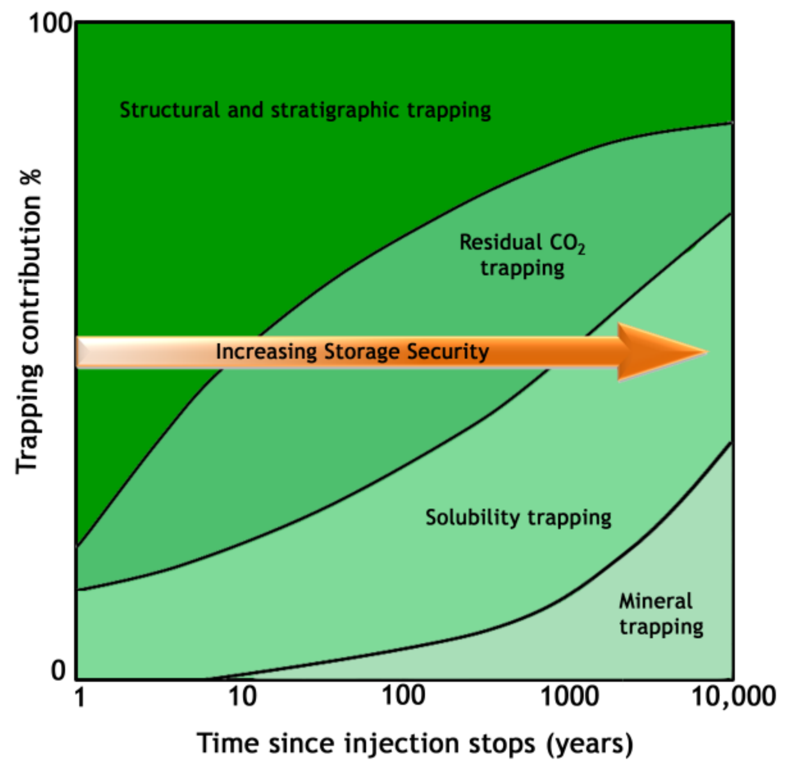
# Science to Inform Geological $CO_2$ Storage Security

**Basic Science → Risk Assessment → Mitigation and Management**




Benson, IPCC, 2007




Modified after Benson et al.2005

# The Energy Frontier Research Centers Aim to Accelerate Discovery Science for Energy Technologies

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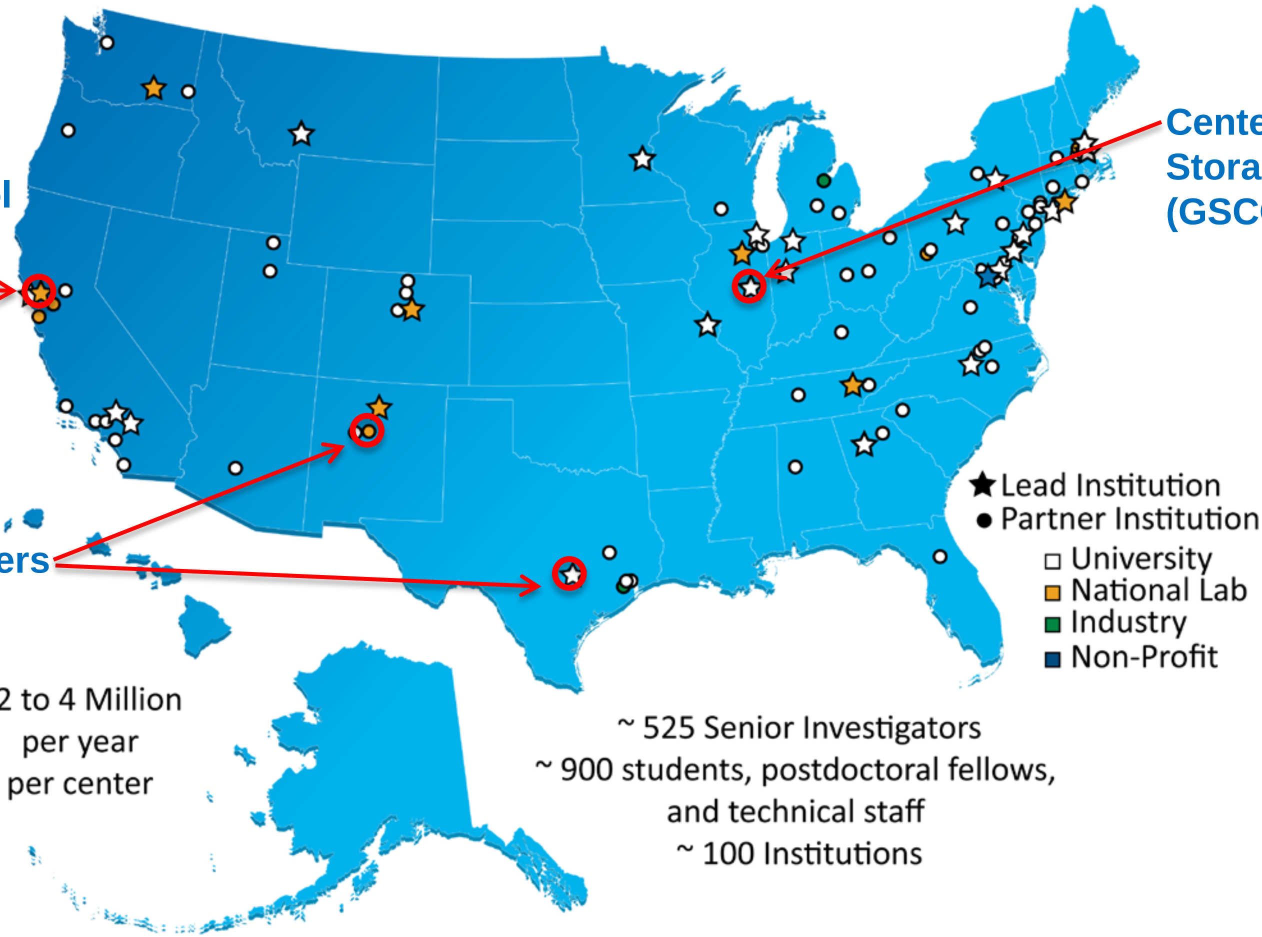
## 32 EFRCs in 32 States + D.C.




**Center for Nanoscale Control of Geologic $CO_2$ (NCGC)**

**Center for Geologic Storage of $CO_2$ ($GSCO_2$)**

**Center for Frontiers of Subsurface Energy Security (CFSES)**

$2 to 4 Million per year per center

~ 525 Senior Investigators
~ 900 students, postdoctoral fellows, and technical staff
~ 100 Institutions

# Center Missions

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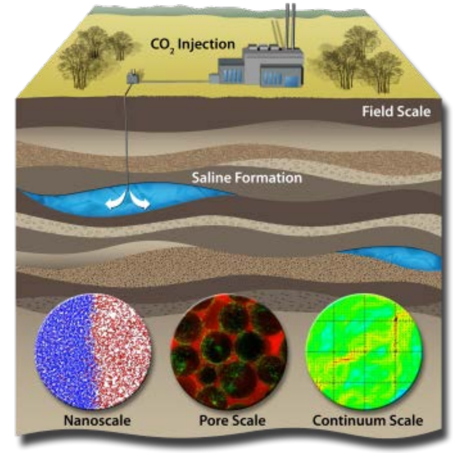
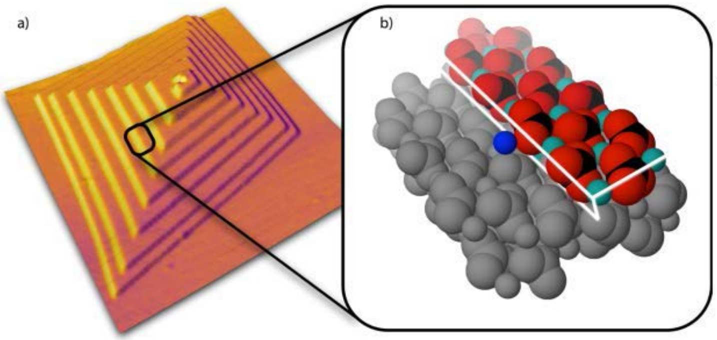
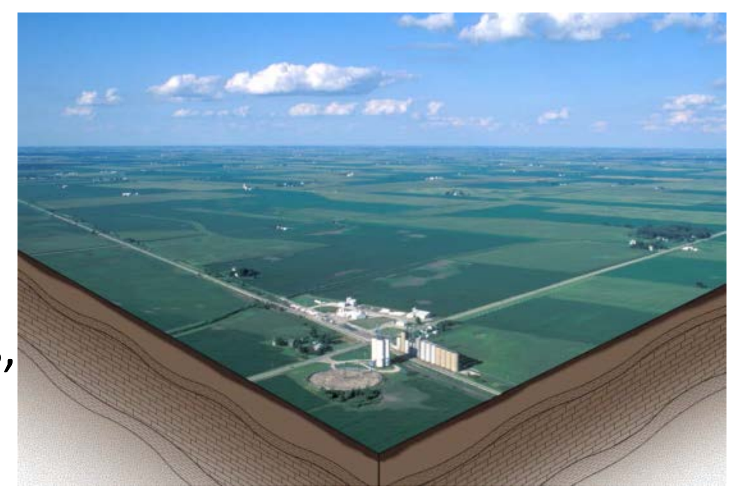



**CFSES:** Understand and control emergent behavior arising from coupled physics and chemistry in heterogeneous geomaterials, particularly during the years to decades time scale.




**NCGC:** 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

**$GSCO_2$:** The goal of this Center is to generate new conceptual, mathematical, and numerical models applicable to reservoir geologic storage systems in specific and strategically identified research areas, based on uncertainty and limitations observed in field pilots and demonstration $CO_2$ injection projects, laboratory experiments, and previous experience of researchers in industry-sponsored applied research.



# CFSES Organizational Structure

Sandia National Laboratories


**EAB**
Steve Bryant
Charles Christopher
Don DePaolo
Derek Elsworth
Robert Finley
Kurt House
Jean Roberts

**Management Team**
Larry Lake – Director
Marianne Walck – Associate Director
Susan Altman, Hilary Olson – Assistant Directors

**Administrative Associate**
Barb Messmore


**THEME 1: FLUID-ASSISTED GEOMECHANICS**
**Theme Leads:**
**Tom Dewers, Sanjay Srinivasan**
M. Balhoff, J. Bishop, P. Eichhbul, N. Espinoza, N. Hayman, M. Hesse, A. Ilgen, M. Martinez, M. Wheeler, H. Yoon

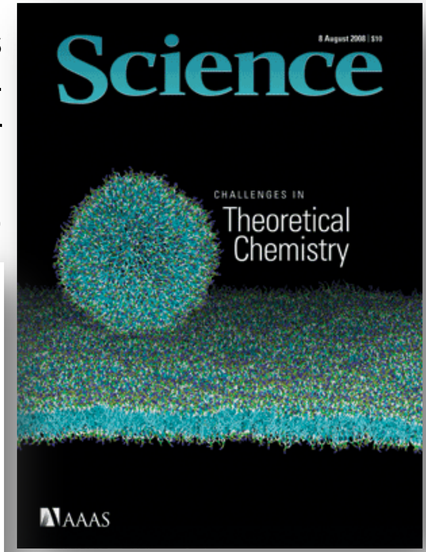

**THEME 2: MULTIFLUID GEOCHEMISTRY**
**Theme Leads:**
**Randall Cygan Marc Hesse**
P. Bennett, B. Cardenas, O. Ghattas, A. Ilgen, C. Tenney, C. Yang


**THEME 3: BUOYANCY-DRIVEN MULTIPHASE FLOW**
**Theme Leads:**
**Tip Meckel, Mario Martinez**
B. Cardenas, D. DiCarlo, N. Espinoza, S. Hovorka, K. Johnston, Y. Wang, H. Yoon, C. Huh


# Examples of CFSES Differentiating Capabilities

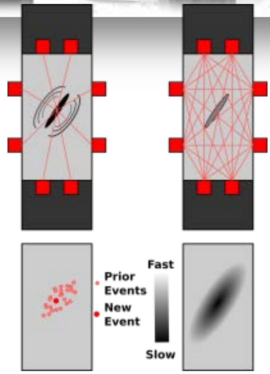
Micro Computed Tomography for imaging of multiphases and contact angles

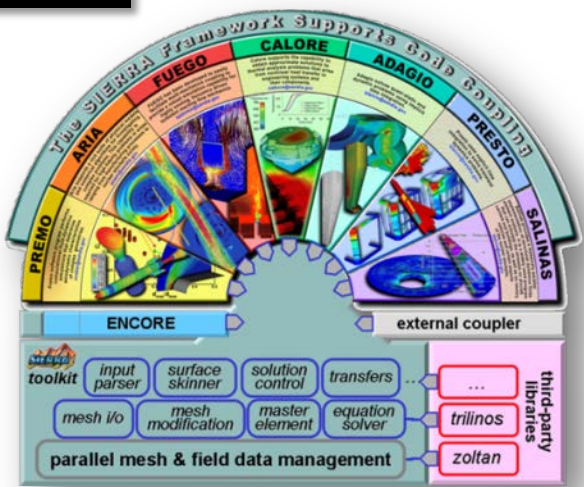
Molecular Dynamics Code LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator)




Red Sky Super Computer


Geomechanical testing for acoustic and ultrasonic imaging of rock deformation




Sierra Mechanics engineering analysis codes

Computed tomography for imaging multi-phase fluid flow through cores

# Chemical and Hydrodynamic Mechanisms for Long-Term Geological Carbon Storage

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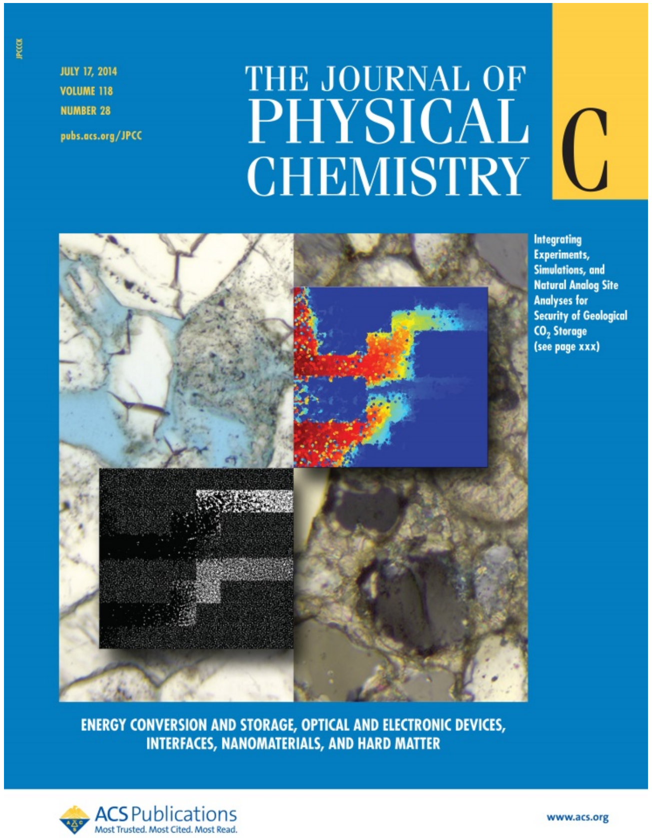


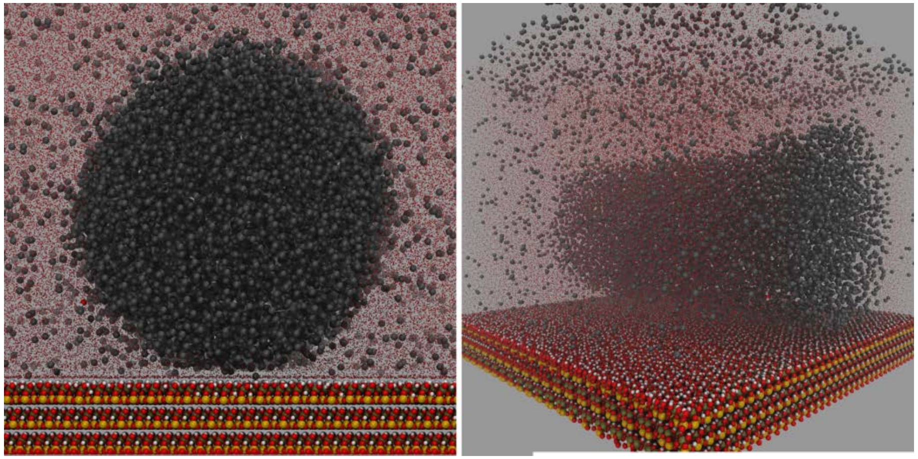

## Scientific Achievement

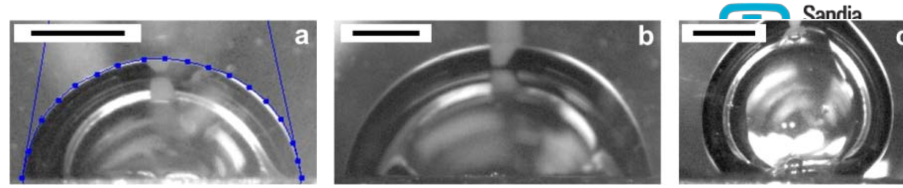
The integration of pore-scale experiments, molecular dynamics simulations, pore-scale simulations, and the study of natural analog sites has provided useful insight in the efficacy of capillary, solubility, dissolution, and mineral trapping for geological $CO_2$ storage (GCS).

## Research Details

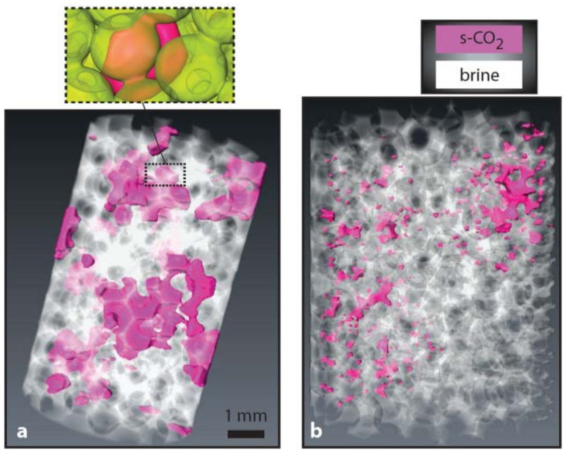
- Nanoscale distribution of wetting and nonwetting phases can differ significantly for different mineral surfaces, impacting macroscopic contact angle measurements
- Indication of strongly hydrophilic media offer significant potential for supercritical $CO_2$ residual capillary trapping
- Nanoparticles, with appropriate surface chemistry, could enable an increase in the overall efficiency of large-scale $CO_2$ storage
- Realistic pore configurations, flow and transport physics, and geochemistry are needed to enhance our fundamental mechanistic explanations of how calcite precipitation alters flow paths by pore plugging to match the Little Grand Wash fault observations

Altman, S.J., et al., 2014. Chemical and Hydrodynamic Mechanisms for Long-Term Geological Carbon Storage. Journal of Physical Chemistry C 118, 15103-15113.

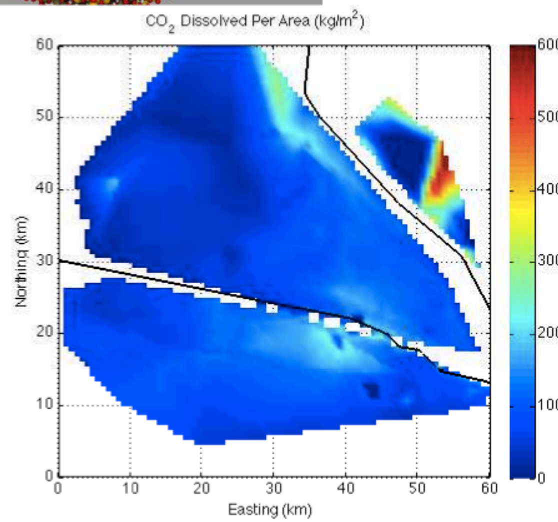




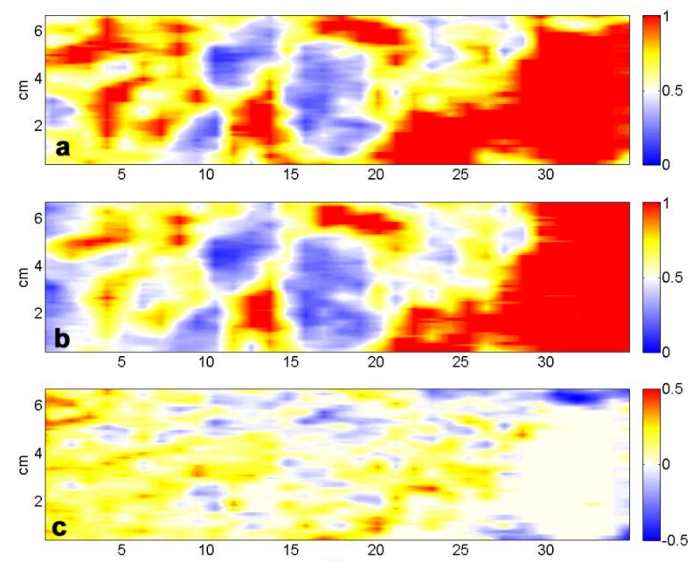

Nanoscale distribution of wetting and nonwetting phases can differ significantly for different mineral surfaces, impacting macroscopic contact angle measurements.




Hydrophobicity of substrate impacts degree of residual trapping (greater trapping with hydrophilic surfaces)




Approximately 22% ± 17% of the initial $CO_2$ emplaced into the Bravo Dome field site of New Mexico has dissolved into the underlying brine.




Surface-treated nanoparticles mitigate coalescence of snapped-off droplets of $CO_2$, controlling wettability and improving storage efficiency

# CFSES Research Impacts Three Challenges to Geologic Carbon Storage

- Sustaining large storage rates, of order gigatons of $CO_2$ per year in the US, for decades without compromising other subsurface resources and without jeopardizing the security with which the $CO_2$ is stored;
- Using pore space with unprecedented efficiency, i.e., placing $CO_2$ so that it occupies half of the reservoir volume, rather than the typical current estimate of less than five percent;
- Controlling undesired or unexpected emergent behavior in the geostorage system, e.g. fracture propagation for unexpectedly long distances, or $CO_2$ plumes channeling through a much smaller volume of the storage reservoir.

# Integrating Research Themes with Challenges

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| | Challenge 1: Sustaining large storage rates | Challenge 2: Using pore space with unprecedented efficiency | Challenge 3: Controlling undesired or unexpected behavior |
|---|---|---|---|
| **Theme 1: Fluid-Assisted Geomechanics** | • Single Fracture propagation and cohesive zone modeling<br>• Phase-field modeling | • Single Fracture propagation and cohesive zone modeling | • Bulk rock strengthening/weakening evaluation |
| **Theme 2: Multifluid Geochemistry** | • Caprock chemical and mechanical stability | • Bravo Dome brine-gas mass transfer<br>• Chemistry at the fluid-fluid interface | • Caprock chemical and mechanical stability<br>• Reactions of $CO_2$ with clay minerals |
| **Theme 3: Buoyancy-Driven Multiphase Flow** | • Meter-scale experiments<br>• Core-scale X-ray CT experiments | • Meter-scale experiments<br>• Core-scale X-ray CT experiments<br>• Mesoscale modeling and invasion-percolation modeling<br>• Ganglion dynamics modeling | • Nanoparticle experiments |

# Fluid Driven Geomechanics

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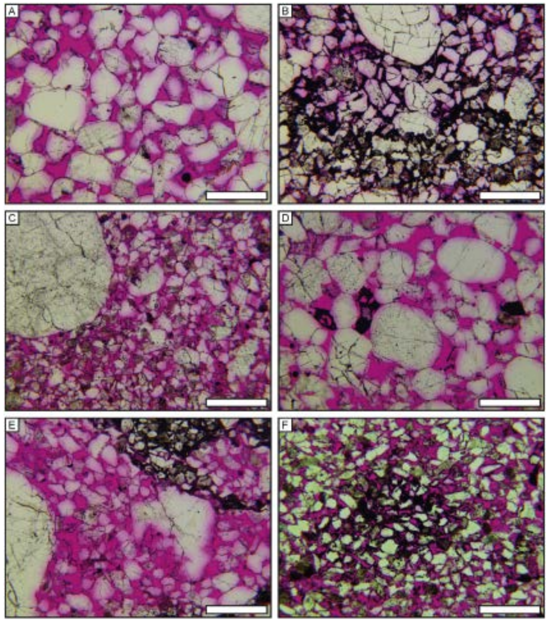
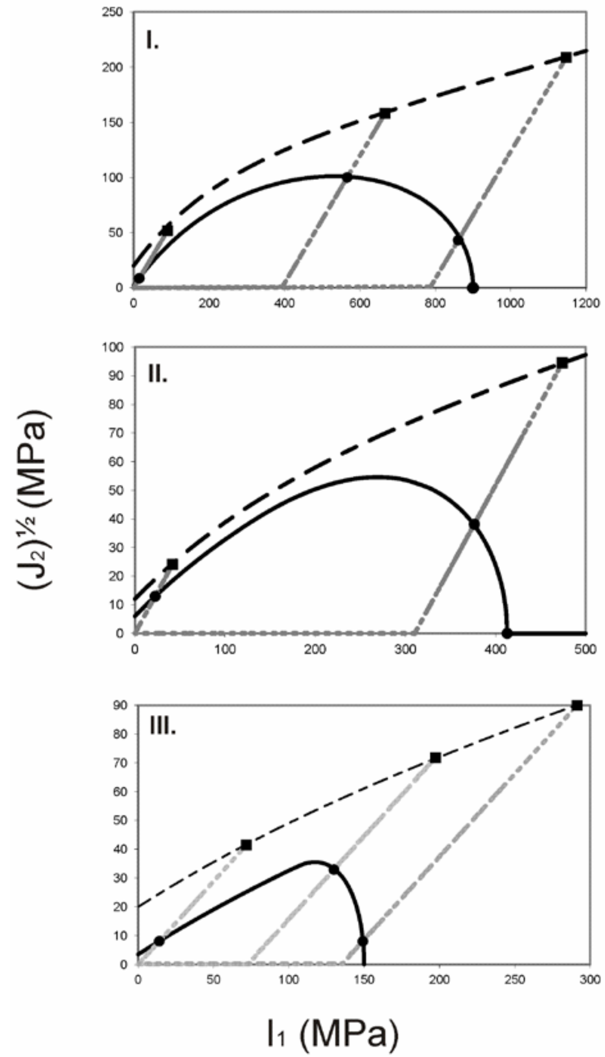







Yield and failure envelope

Dewers, T.A., Newell, P., Broome, S., Heath, J., Bauer, S., 2014. Geomechanical behavior of Cambrian Mount Simon Sandstone reservoir lithofacies, Iowa Shelf, USA. International Journal of Greenhouse Gas Control 21, 33–48.

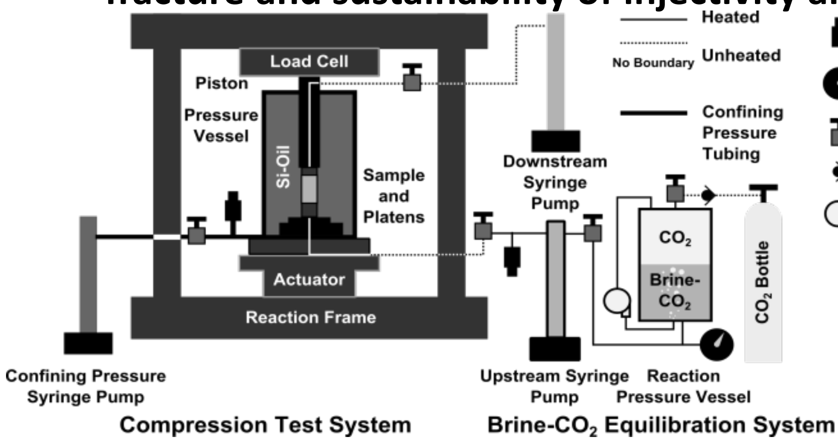
# Mechanical variability and chemo-mechanical constitutive behavior of Gulf Coast, US Reservoirs

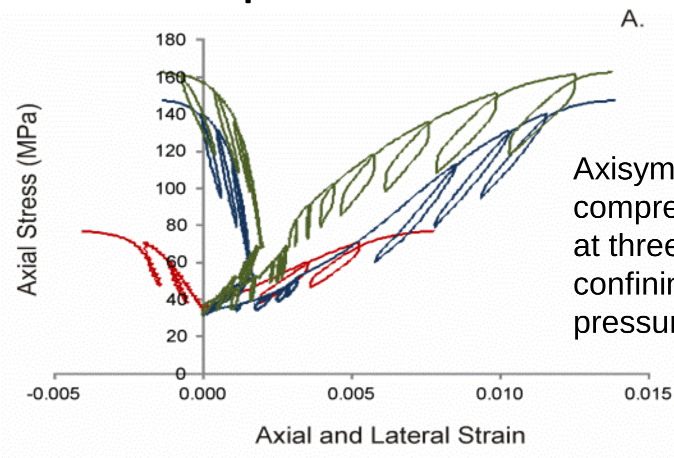
## Scientific Achievement

- Performed rock mechanics experiments at *in situ* conditions for Geologic Carbon Storage (GCS)
- Show certain sandstone reservoirs are susceptible to weakening, creep, and fracture resulting from chemical perturbation associated with $scCO_2$ injection
- Developed constitutive model linking elasto-plastic, creep, and fracture response to chemical conditions and reservoir heterogeneity

## Significance and Impact

1) Cenozoic and Mesozoic US gulf coast clastic sequences appeal ideal for GSC (injectivity, storage efficiency and security)
2) Explanation for "leak-off" behavior at Seacarb Cranfield injection site
3) Show that chemical manipulation of injectate could provide a viable path for subsurface control of fracture and sustainability of injectivity and sweep

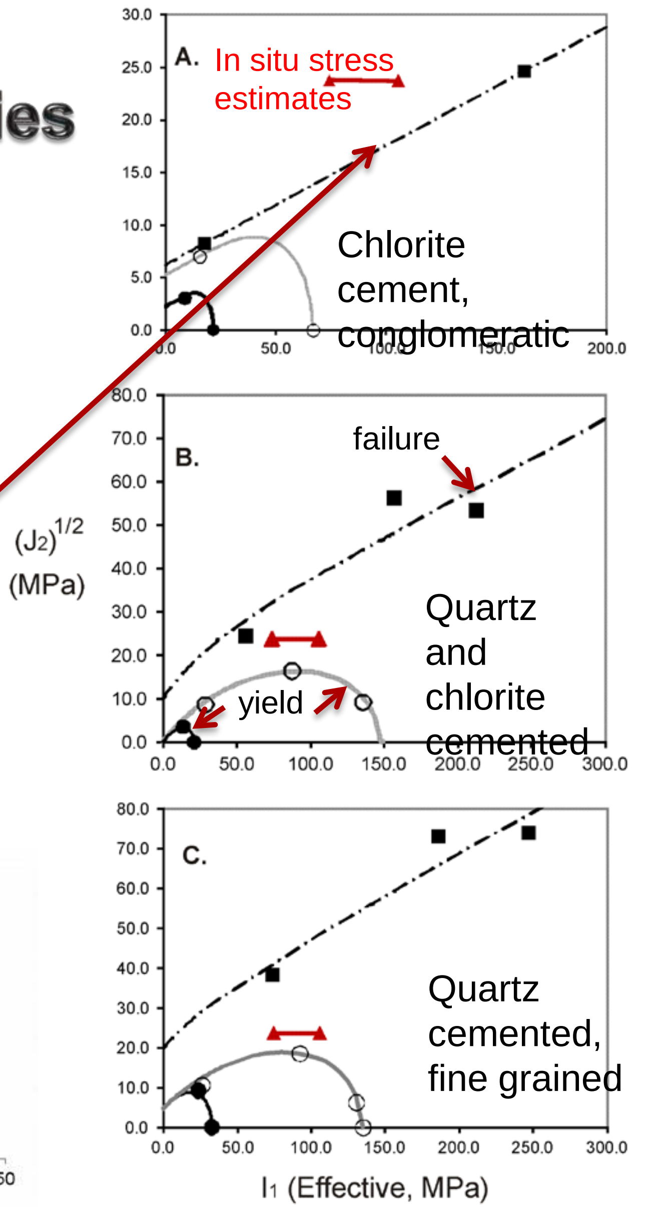


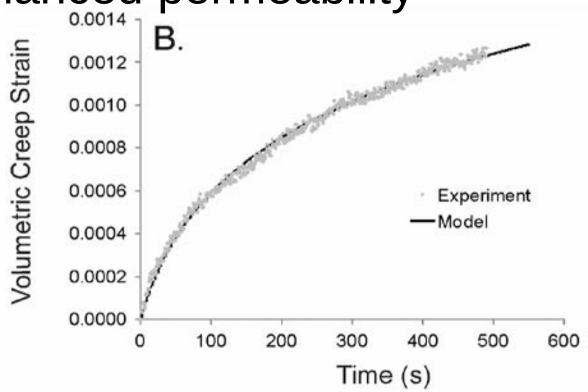



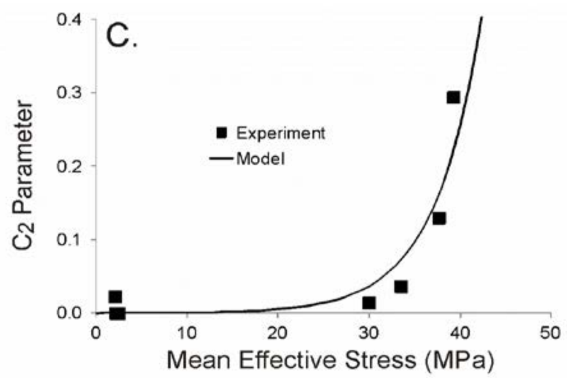

Axisymmetric compression at three confining pressures

# $CO_2$ injection changes deformation behavior of certain rock types of lithofacies

- Simulated chemical conditions during scCO2 injection produce heightened creep response, degradation of elastic moduli (and thus seismic velocities), lower yield and failure envelopes for three facies of the lower Tuscaloosa Formation, US Gulf Coast
- Chlorite cemented lithofacies are particularly vulnerable
- Lowered failure envelope can induce a “self-shearing”, improving injectivity and sweep efficiency
- Accelerated creep may limit lifetime of shear-enhanced permeability



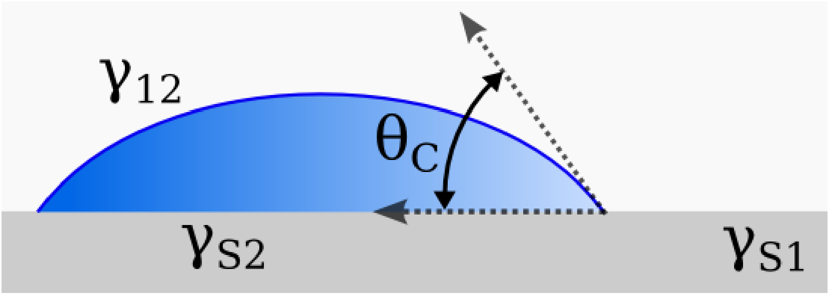

Primary and secondary creep follow log law with exponential stress dependence

Mechanical variability and constitutive behavior of the lower Tuscaloosa Formation supporting the SECARB Phase III $CO_2$ Injection Program, Alex Rinehart, Pania Newell, Scott Broome, and Thomas Dewers, *AAPG Bulletin* **2014** *, submitted*

# Multifluid Geochemistry

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

- **interfacial tension $\gamma_{12}$**
  - **surface free energy**
- **contact angle $\theta_C$**
  - **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)**

# Pioneering Molecular Dynamics

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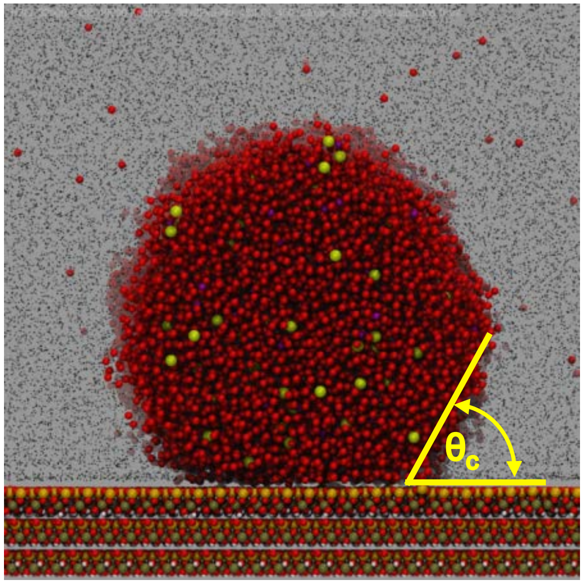
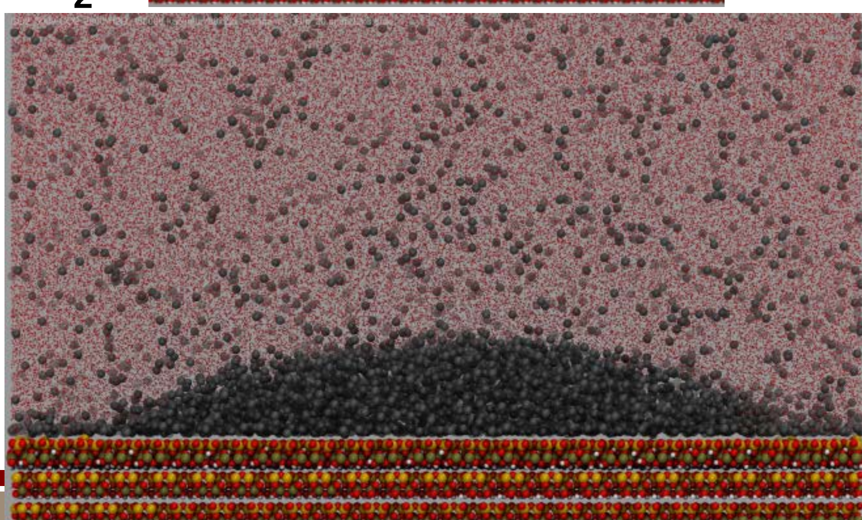
## Hydrophobic
**kaolinite (siloxane-like) surface**

**0.7M NaCl in $CO_2$**

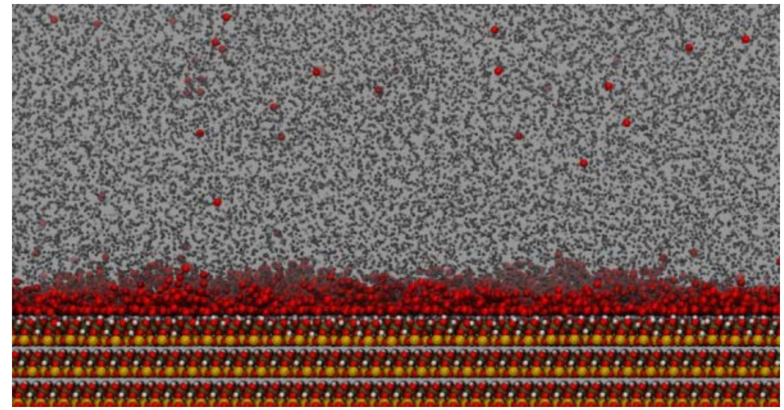



**$CO_2$ in $H_2O$**

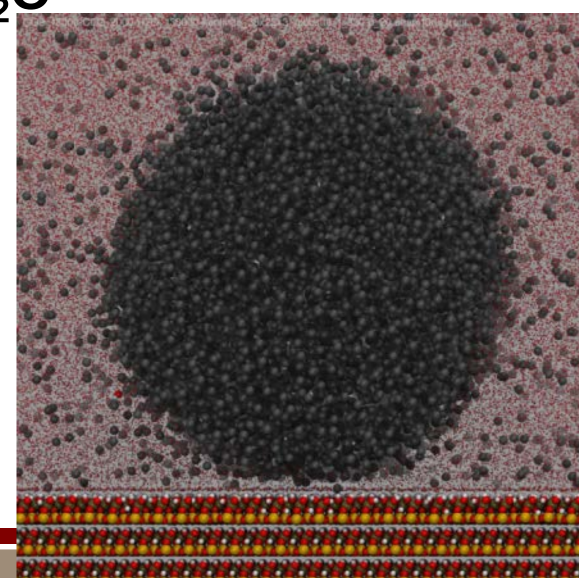


## Hydrophilic
**kaolinite (gibbsite-like) surface**

**$H_2O$ in $CO_2$**



**$CO_2$ in $H_2O$**

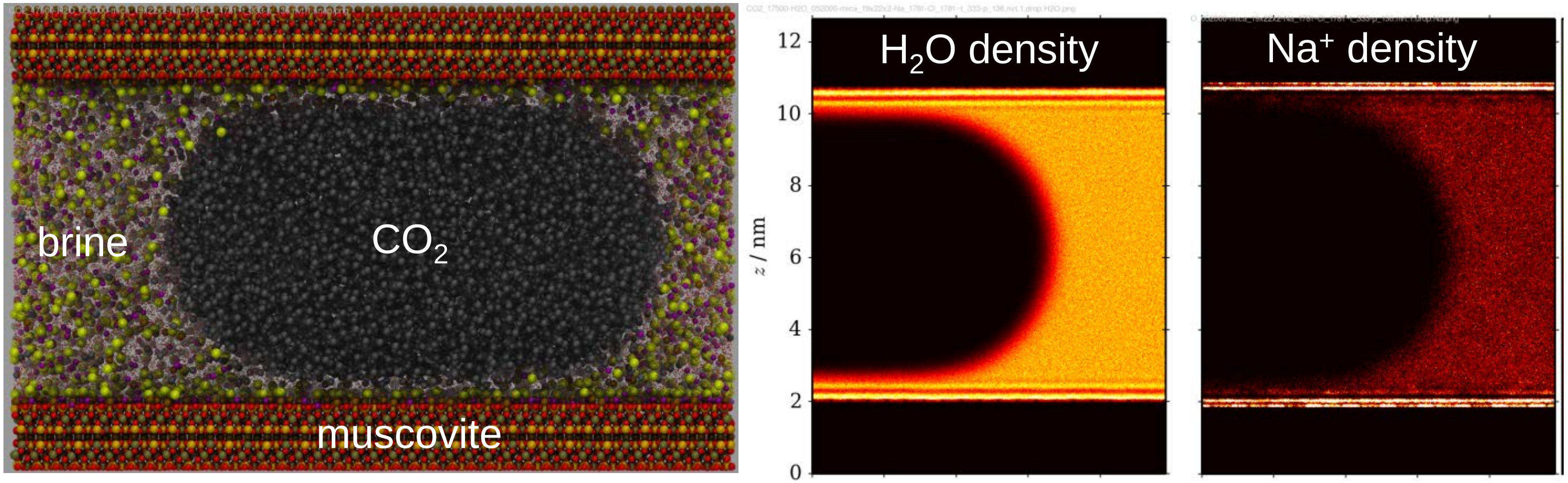


Tenney, C.M., Cygan, R.T., 2014.. Environmental Science & Technology 48, 2035-2042.

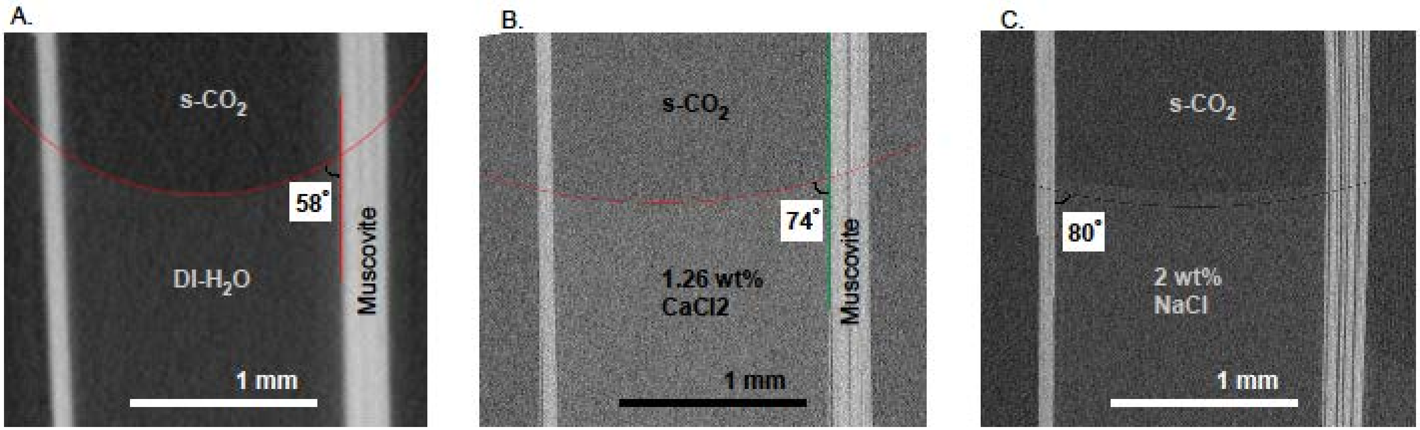
Cygan, Romanov, and Myshakin, *Journal of Physical Chemistry C*, 2012.

# Pioneering Molecular Dynamics

Simulation: supercritical $CO_2$ and brine wetting in mineral nanopores

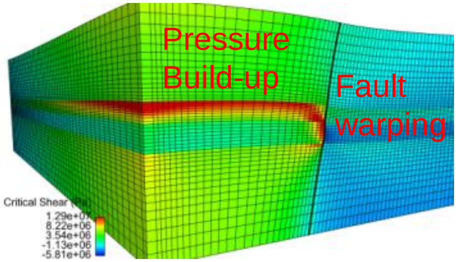


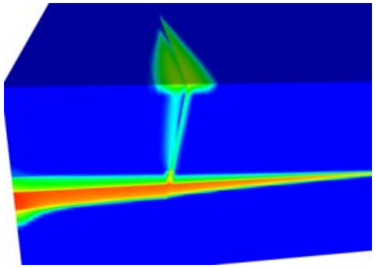

Experiment: high-resolution micro X-ray CT scanning of $CO_2$/brine/mineral interface



# Modeling Fluid-Induced Geomechanics

## Impact of faults on critical shear failure and leakage

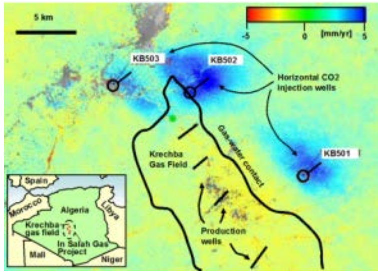


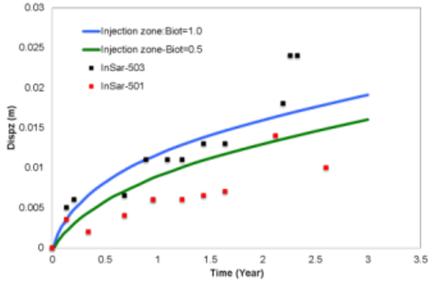



**Low permeability** fault impedes $CO_2$ injection and builds pressure behind the fault, inducing critical shear failure in both the caprock and fault.

**High permeability** fault creates a pathway for leakage of $CO_2$ through the caprock.

## In Salah Investigation

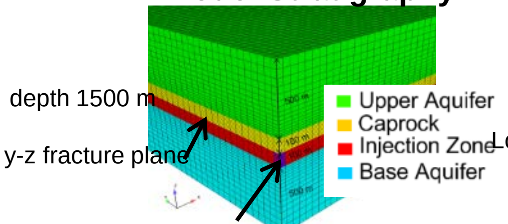


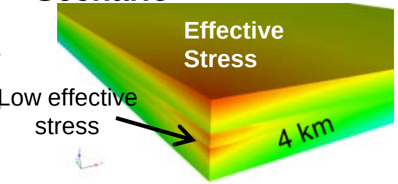

**Impact of geomechanical and hydrological properties on injection-induced uplift at InSalah**

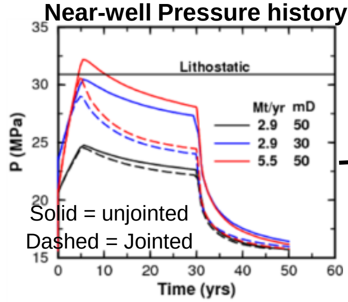
## Jointed Rock Model

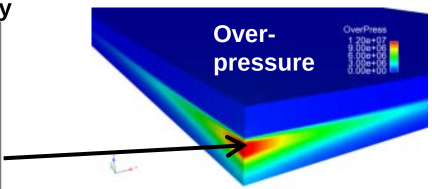
### Model Stratigraphy




### Damaged Caprock Scenario




**High injection rates and/or low storage aquifer permeability can lead to fracturing of the caprock, inducing leakage.**

Bishop et al., ARMA 12-190 (2012)
MJ Martinez et al., Int. J. Greenhouse Gas Control, 17, 148-160 (2013)
Turner, et al., (2014) Int. J. Geomech., DOI: 10.1061(ASCE)GM.1943-5622.0000416.
Newell, et al., Systematic Investigation of the Influence of Geomechanical and Hydrogeological Properties on Surface Uplift at In Salah, (2015)submitted.

# Estimating solubility trapping rates

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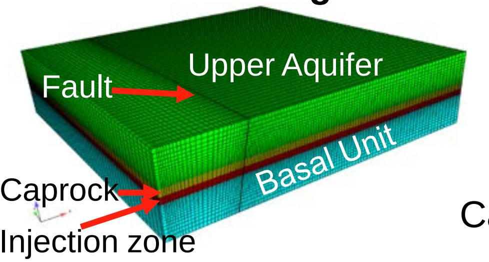
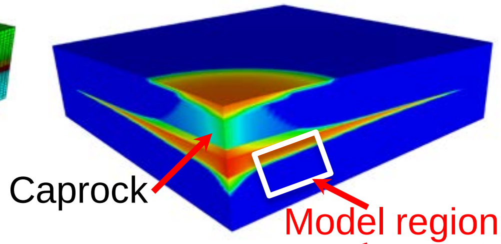
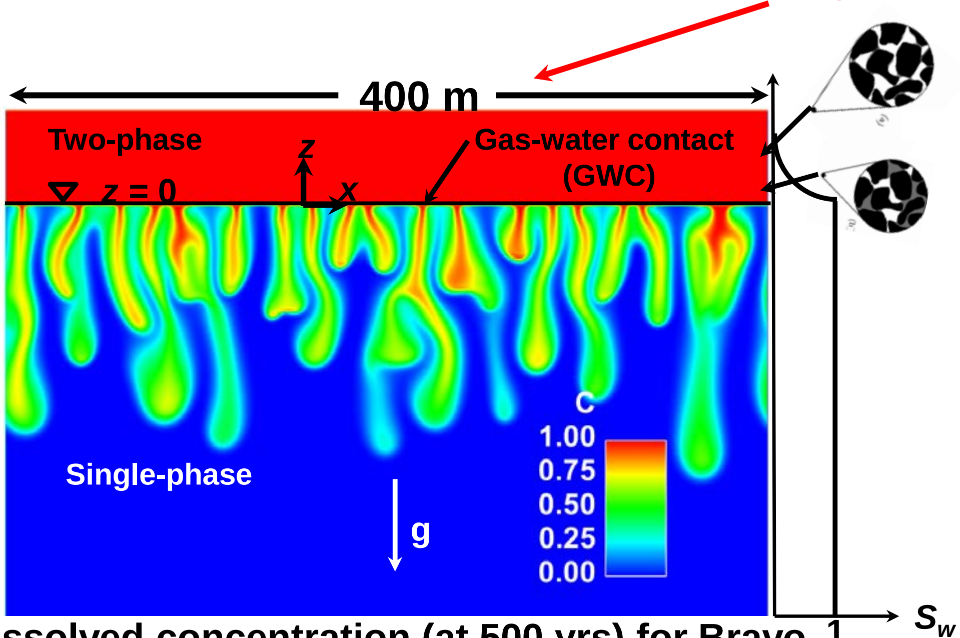
Discrete Geologic Model




Injection with leaky caprock




**Dissolved concentration (at 500 yrs) for Bravo Dome properties with 50 kPa entry pressure.**

## Scientific Challenge

- Solubility trapping is a critical mechanism in geologic carbon storage
- Buoyantly driven convective dissolution enhances the rate of dissolution, but is difficult to quantify in the field
- Theory and computational models have heretofore ignored the two-phase region above the gas-water contact where dissolution actually takes place

## Impact and Significance:

- Our two-phase model predicts dissolution rates > 3 times higher than previous estimates.
- The dissolution rate increases with capillary wicking potential (entry pressure) via convective current loops penetrating above the gas-water contact.
- An upper bound may be 5x based on a mixing model analog

# DOE Crosscutting "Tech Teams": Subsurface Technology and Engineering RD&D (SubTER)

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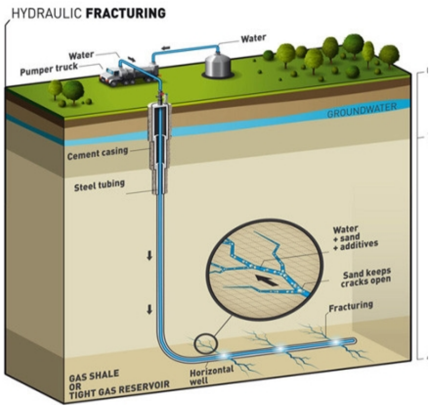
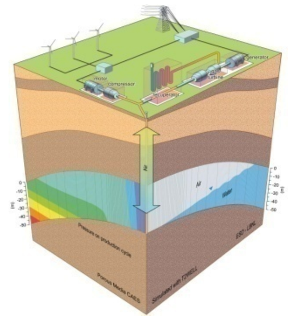
## "Adaptive Control" of subsurface fractures and flow

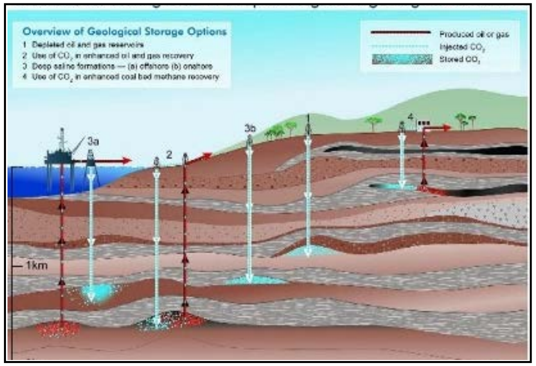
Ability to adaptively manipulate – rapidly and with confidence - subsurface fracture length, aperture, branching, connectivity and associated reactions and fluid flow.




Fractures by Design: Control fracture length & branching patterns in real-time

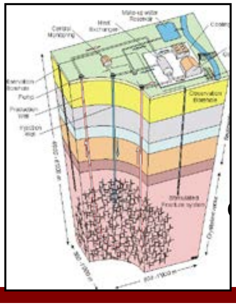


Compressed Air Energy Storage

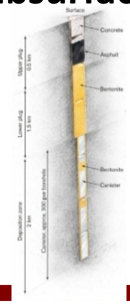


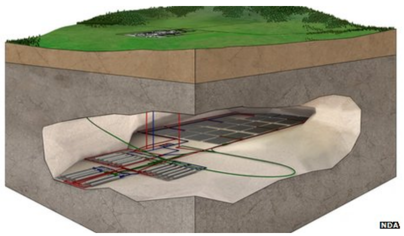

Carbon Sequestration: Enhance injectivity, optimize storage, plug leakage pathways

Enhanced geothermal energy



Safe subsurface storage of nuclear waste





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# Questions?

CFSES

Center for Frontiers of Subsurface Energy Security

# Backup Slides

# Relevant CFSES References


- Residual Trapping
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  - Mehmani, Y.; Balhoff,M. T. Bridging from Pore to Continuum: A Hybrid Mortar Domain Decomposition Framework for Subsurface Flow and Transport. Multiscale Model. Simul., 2014, 12, 667-693.

<table>
<tr><th>CFSES</th><th>Challenge 1: Sustaining Large Storage Rates</th><th>Challenge 2: using pore space with unprecedented efficiency</th><th>Challenge 3: controlling undesired or unexpected behavior</th></tr>
<tr><td rowspan="2">Theme 1: Fluid-Assisted Geomechanics</td><td>Single fracture propagation and cohesive zone modeling (SNL: Dewers, Bishop, Martinez, Yoon; UT: Eichhubl)</td><td rowspan="2">Single fracture propagation and cohesive zone modeling (SNL: Dewers, Bishop, Martinez, Yoon; UT: Eichhubl)</td><td rowspan="2">Bulk rock strengthening/weakening evaluation (SNL: Dewers, Ilgen; UT: Espinoza)</td></tr>
<tr><td>Phase field modeling (UT: Wheeler, Srinivasan, Song Lee, Hayman, Reber)</td></tr>
<tr><td rowspan="3">Theme 2: Multifluid Geochemistry</td><td rowspan="3">Caprock chemical and mechanical stability (SNL: Ilgen)</td><td>Bravo Emplacement Rates (UT: Hesse, Ghattas, TBD PostDoc)</td><td>Caprock chemical and mechanical stability (SNL: Ilgen)</td></tr>
<tr><td>Bravo Dome Gas Composition Dynamics (UT: Hesse, Larson, Yang, TBD Grad)</td><td rowspan="2">Reactions of $CO_2$ with clay minerals (SNL: Cygan, Ilgen, Tenney, TBD Postdoc (Ilgen), TBD Postdoc (Tenney); UT: Bennett, Cardenas, Guiltinan)</td></tr>
<tr><td>Geochemistry at the fluid-fluid interface (SNL: Cygan, Tenney, TBD Postdoc; UT: Bennett, Cardenas, Guiltan, TBD Cardenas Postdoc, TBD Bennett Grad)</td></tr>
<tr><td rowspan="4">Theme 3: Buoyancy-Driven Multiphase Flow</td><td rowspan="3">Meter-scale experiments (SNL: Yoon, TBD Post-doc; UT: Meckel, DiCarlo, TBD Grad)</td><td>Meter-scale experiments (SNL: Yoon, TBD Post-doc; UT: Meckel, DiCarlo, TBD Grad)</td><td rowspan="4">Nanoparticle experiments (UT: DiCarlo, Huh, Johnston. Roy Wong)</td></tr>
<tr><td>Micro X-ray CT experiments (UT: Cardenas, Espinoza)</td></tr>
<tr><td>Invasion-percolation modeling (UT: Meckel, Hovorka, Prasanna K., TBD)</td></tr>
<tr><td>Micro X-ray CT experiments (UT: Cardenas, Espinoza)</td><td>Ganglion Dynamics modeling (SNL: Martinez, Wang, Yoon, TBD Postdoc; UT: Hovorka)</td></tr>
</table>

# How Can the Academic Community Be Involved?

- **Your input now can contribute to shaping the scope of SubTER.**
- **Funding opportunities will be announced leading up to and/or after the full launch of this initiative in FY16 (pending appropriations).**
- **Partnerships with National Labs can facilitate involvement in other aspects of the Subsurface Crosscut starting in FY15.**

## Subsurface Working Team: 13 Laboratories

# Subsurface Control for a Safe and Effective Energy Future

## Adaptive Control of Subsurface Fractures and Fluid Flow

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| Wellbore Integrity & Drilling Technologies | Subsurface Stress & Induced Seismicity | Permeability Manipulation | New Subsurface Signals |
|---|---|---|---|
| Improved well construction materials and techniques | Measurement of stress and induced seismicity | Physicochemical fluid-rock interactions | New sensing approaches |
| Autonomous completions for well integrity modeling | Manipulation of stress and induced seismicity | Manipulating flowpaths | Integration of multi-scale, multi-type data |
| New diagnostics for wellbore integrity | Relating stress manipulation and induced seismicity to permeability | Characterizing fractures, dynamics, and flows | Adaptive control processes |
| Remediation tools and technologies | Applied risk analysis of subsurface manipulation | Novel stimulation methods | Diagnostic signatures and critical thresholds |
| Fit-for-purpose drilling and completion tools (e.g. anticipative drilling, centralizers, monitoring) | | | |
| HT/HP well construction / completion technologies | | | |

**Energy Field Observatories**

**Fit For Purpose Simulation Capabilities**