SAND2014-19138PE

DOE OFFICE OF SCIENCE – BES GEOSCIENCE RESEARCH AT SANDIA

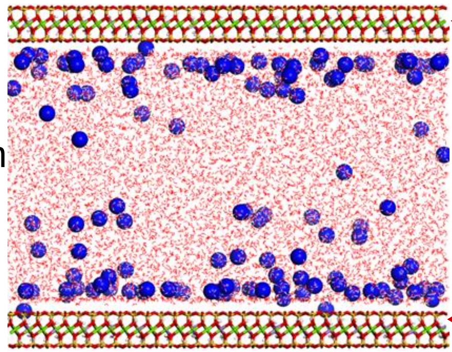
NOVEMBER 2014

Geochemistry: The nature of the mineral-water interface

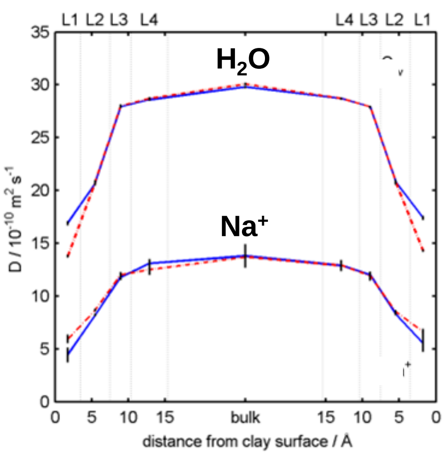
Personnel
Randy Cygan PI
Jeff Greathouse PI
Louise Criscenti PI
Anastasia Ilgen PI
Collaborators: Texas, MSU, Ohio State

Task 1: Complex Clay Interfaces

sodium ions

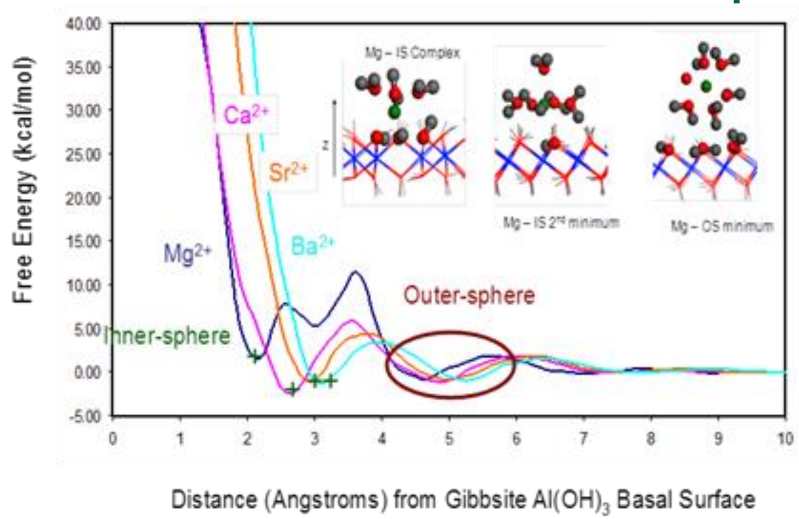


charged clay surfaces



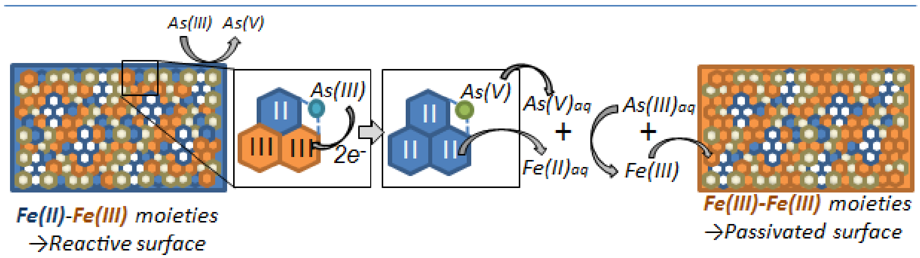
- Molecular modeling of interfacial structure and diffusion in a clay pore

Task 2: Alkaline Earth Metal Adsorption



- Development of thermodynamic models for contaminant adsorption using molecular simulation

Task 3: Redox on Clay Mineral Surfaces



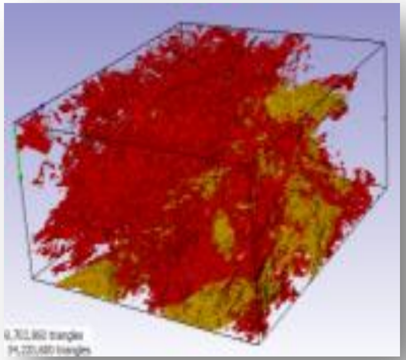
- Experimental and spectroscopic studies to develop a mechanistic model of the clay structural iron reactivity

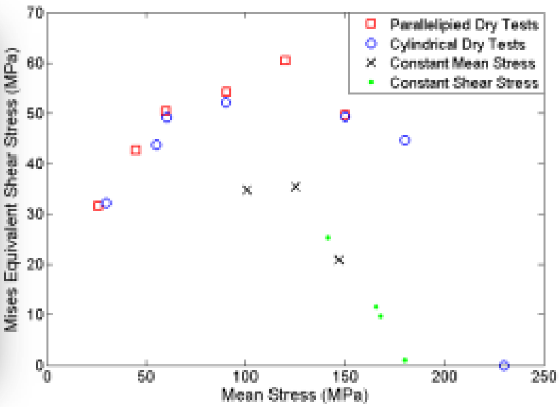
Geomechanics: Heterogeneous deformation of porous media

(SNL PIs:Tom Dewers, Kate Klise, and Steve Bauer)

Objective

To investigate non-Darcian flow, and coupled constitutive behavior of heterogeneous, deforming porous media





Tasks

I. Mudstone (Shale) multiphysics

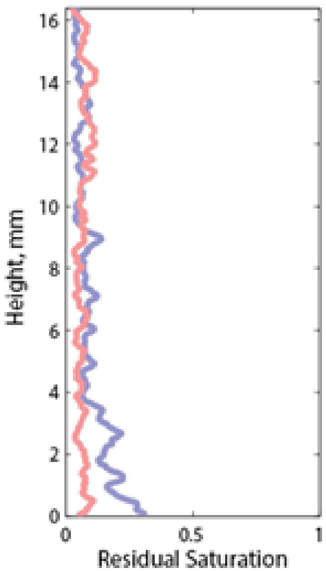
- FIB/SEM reconstructed 3D nano-pore network in Haynesville shale.

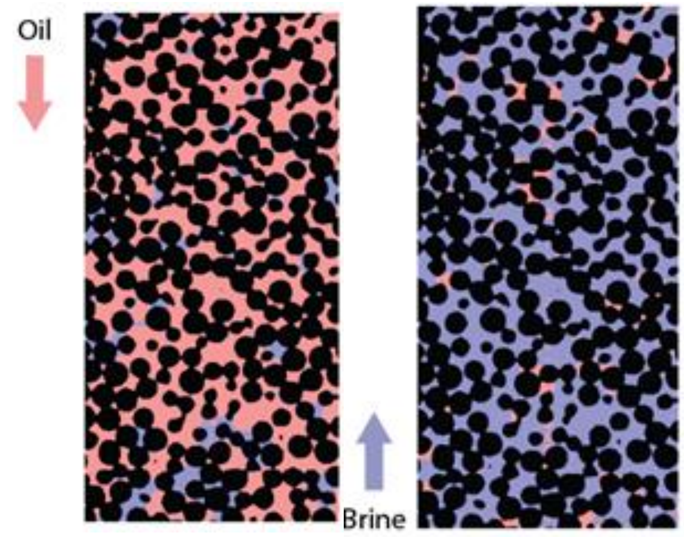
II.Multiphase Flow under varying wettability & pressure

- Multiphase flow experiments using CT imaging under glass/glass-coated bead packing

III.Testing Paradigms of Poroplasticity

- Constant shear stress vs constant mean stress





Shale Poromechanics: Heterogeneity, Flow, Failure, and Creep

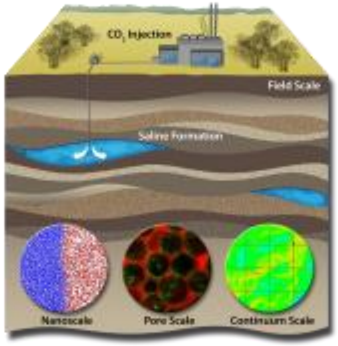
PI:Thomas Dewers (SNL) , co-PIs: Hongkyu Yoon (SNL) and Zuleima Karpyn (PSU)

	Methodologies: Multiscale characterization	Objectives: Fundamental understanding of shale for subsurface applications
Task 1: Shale Mechanics Across Scales	• Micropillar nanoindentation at pore-grain scale (10nm to 10μm) • True-triaxial testing with ultrasonics at macroscale (1”-4” core samples) • Deformation partitioning with in-situ neutron methods	• Anisotropy, elasticity and strength across scales • REV scale for shale poro-mechanics • Constitutive law based on in-situ neutron testings for microscale shale behaviors
Task 2: Transport Modeling with Experimental Validation	• Multiscale imaging across scales (CT, confocal, FIB-SEM, TEM, EDS) • Measurement of effective-stress dependent permeability and sorption • Coupled chemo-mechanical fluxes • Pore scale modeling of gas transport	• Multiscale digital rock physics for shale topology and lithofacies • Coupled poroelastic and sorption effects on permeability • Gas and fluid flows in nano-confined pore geometry
Task 3: Creep Response at In-situ Conditions	• Long term creep tests at elevated temperature with stress-stepping • Imaging analysis of pore-scale microstructural consequences of creep	• Deformation partitioning between organic-rich, clay-rich, and other components of shale microlithofacies • Development of constitutive creep models for shale lithofacies that are tied to pore-scale textural evolution

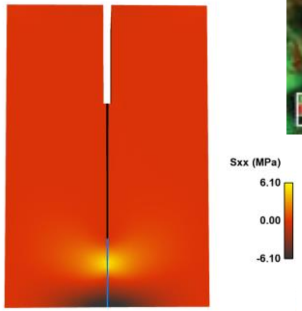
Center for Frontiers of Subsurface Energy Security – Energy Frontier Research Center

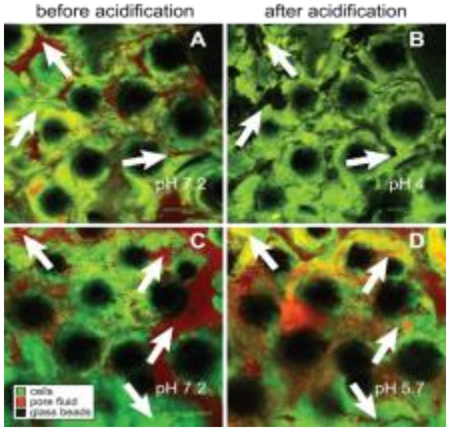
Goal

To understand and control emergent behavior arising from coupled physics and chemistry associated with carbon sequestration in heterogeneous geomaterials.



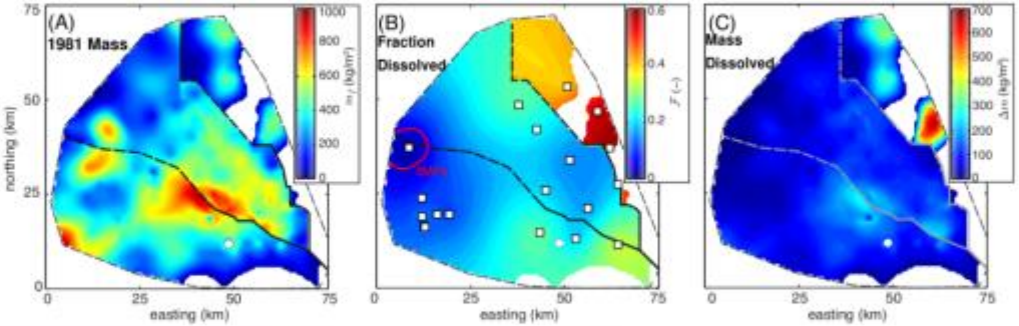
Established synergistic experimental and modeling capability for the science of fluid-driven geomechanics





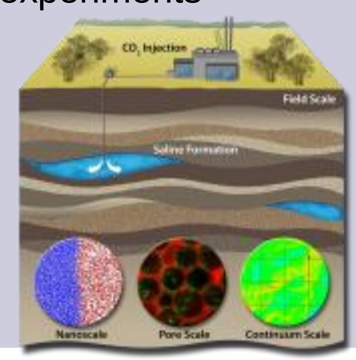
Provided new insight on the impact of GCS on subsurface microbial communities and the subsequent impact on the chemical environment

Provided new data and new insight into the controls on long-term dissolution of stored CO_2



Center for Frontiers of Subsurface Energy Security – Energy Frontier Research Center

	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	• Crack-tip chemo-mechanics • Phase-field modeling	• Cohesive zone modeling • Fracture network analog sites	• Bulk rock weakening evaluation • Influence of chemistry in frictional slip (Crack-tip chemo-mechanics)
Theme 2: Multifluid Geochemistry	• Crack-tip chemo-mechanics	• Bravo Dome brine-gas mass transfer • Chemistry at the fluid-fluid interface	• Crack-tip chemo-mechanics • Reactions of CO_2 with clay minerals
Theme 3: Buoyancy-Driven Multiphase Flow	• Meter-scale experiments • Core-scale X-ray CT experiments	• Meter-scale experiments • Core-scale X-ray CT experiments • Mesoscale modeling and invasion-percolation modeling • Ganglion dynamics modeling	• Nanoparticle experiments



TEXAS CFSES Sandia National Laboratories

Highlight Slides

Molecular Simulation of Organic Dye Molecules at the Mineral-water Interface

Scientific Achievement

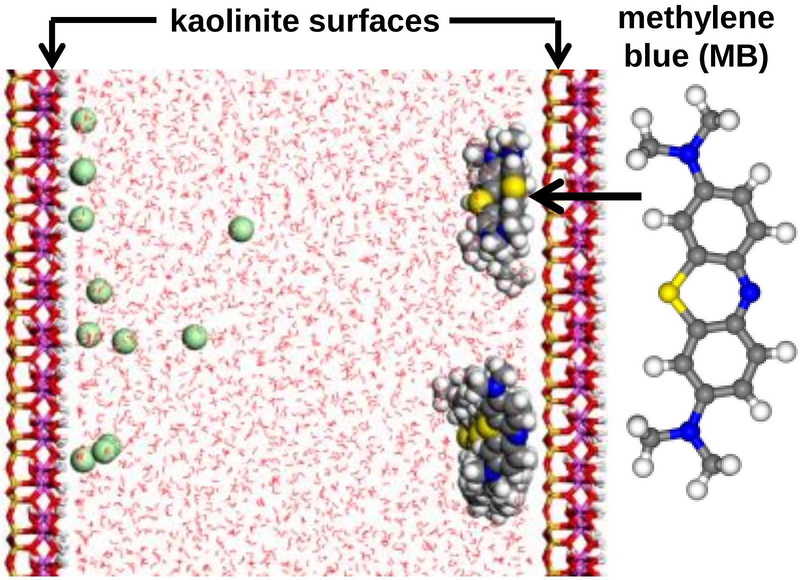
We can predict the structural and thermodynamic properties of organic dyes such as methylene blue (MB) on clay mineral surfaces, in agreement with experiment.

Significance and Impact

Understanding how organic dyes adsorb on clay surfaces aids in the characterization of unknown mineral phases based on MB spectroscopy.

Research Details

- **Classical simulations of hybrid mineral-organic systems were validated by comparison with high-level quantum calculations.**
- **At high concentration, strong hydrophobic interactions cause MB dimers and higher aggregates to form, in agreement with experiment.**
- **Review paper on mineral interactions with natural organic matter written as part of international fellowship (Greathouse, Durham University UK).**



MB adsorption in a kaolinite pore. Partitioning of MB cations at the hydrophobic siloxane surface and chloride anions at the hydrophilic aluminol surface.

Greathouse, J.A., Johnson, K.L., and Greenwell, H.C. (2014) Interactions of natural organic matter with layered minerals: Recent developments in computational methods at the nanoscale. ***Minerals***, *4*, 519-540.

Greathouse, J.A. et al. (2014) Methylene blue adsorption on the basal surfaces of kaolinite: Structure and thermodynamics from quantum and classical molecular simulation. ***Clays and Clay Minerals***, submitted.

Pore-scale multiphase flow experiments reveal the details of hydrocarbon distribution in porous media

Scientific Achievement

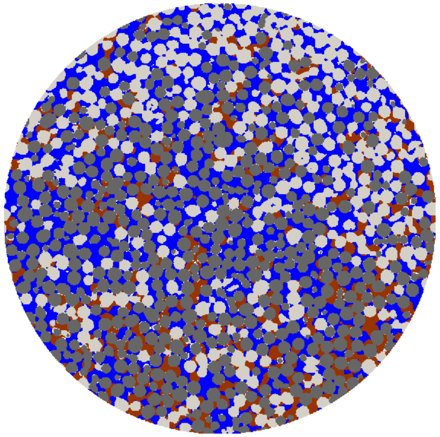
Observing multiphase flow at the pore scale reveals the effects of wettability and confining pressure on sweep efficiency and residual oil and water distributions in porous materials

Significance and Impact

Different wettabilities lead to different displacement mechanisms at the pore scale, resulting in different contact angles (significant implications for CO_2 sequestration, EOR)

Research Details

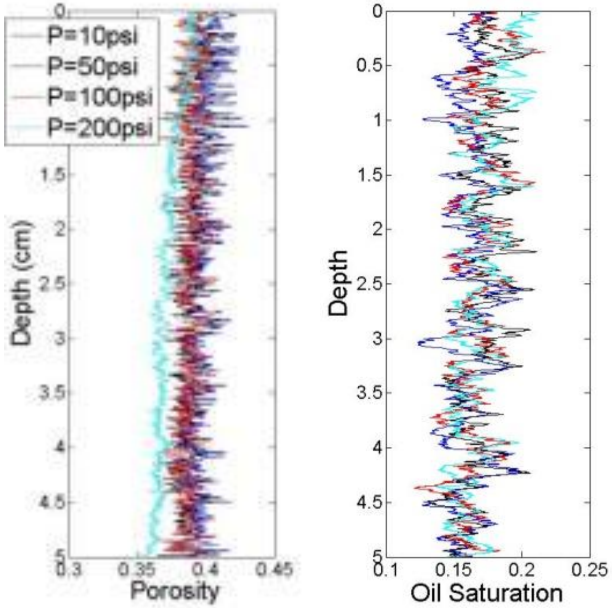
- X-ray microtomography (CT) reveals pore-level details of wettability and the distribution of oil and water phases
- Compaction is observed by porosity change at 200 psi and residual oil saturation becomes more homogeneous after multiple drainage and imbibition cycles



Residual saturation profiles and CT cross section using glass and plastic beads,

10 mm

Glass bead
Plastic bead
Oil
Brine



Porosity and oil saturation profiles

J.G. Celauro, V.A. Torrealba, Z.T. Karpyn, K.A. Klise, S.A. McKenna (2014), Pore-scale multiphase flow experiments in bead packs of variable wettability. Geofluids, 14(1), 95-105