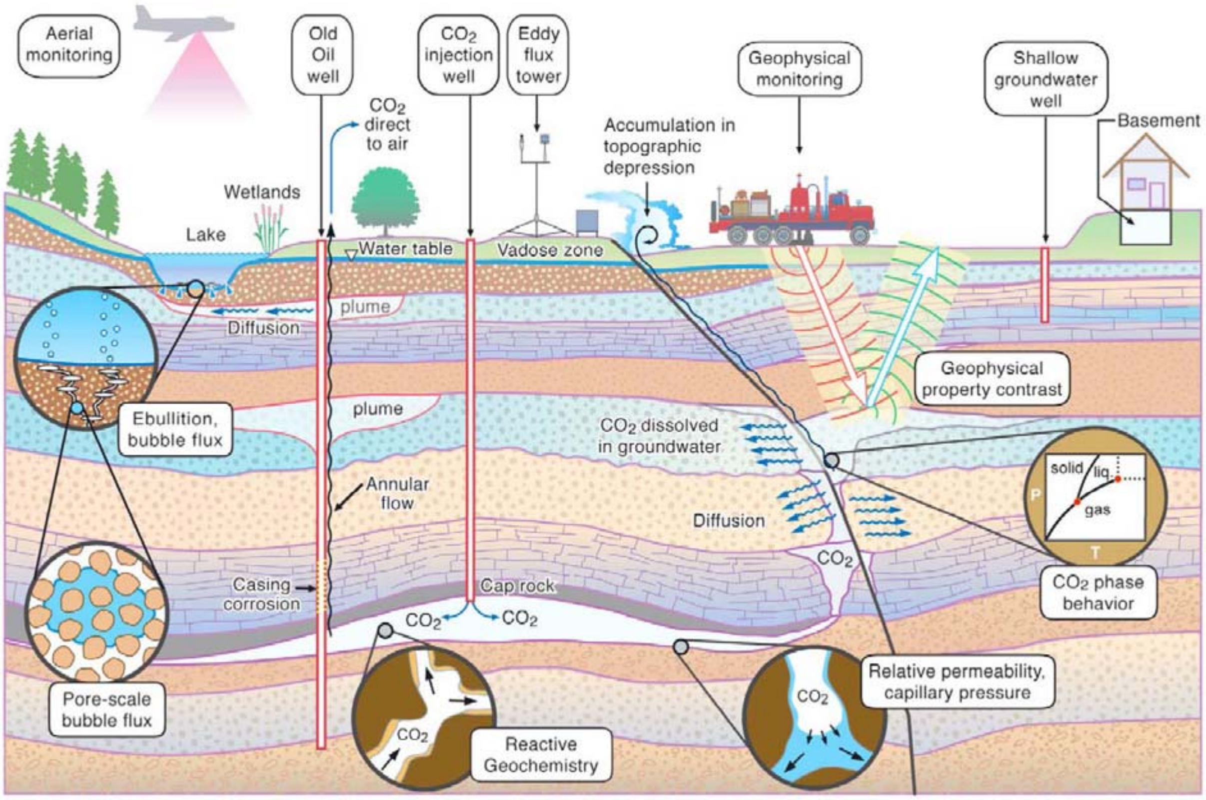
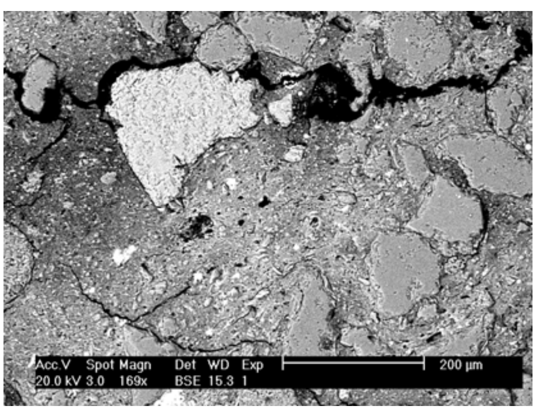
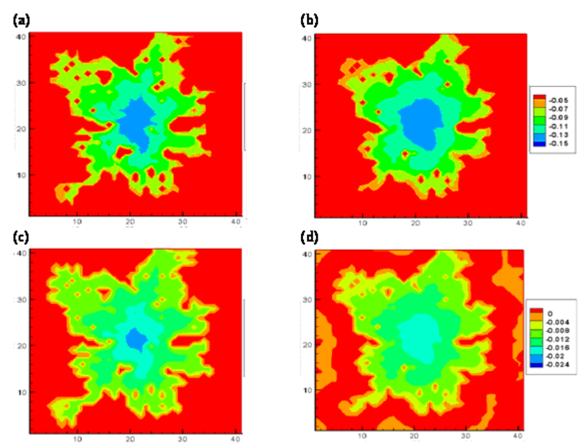


Basic Research Relevant to Geological CO_2 Sequestration





March 12-14, 2008

Geosciences Research Program, Office of Basic Energy Sciences

FORWARD

"Basic Research Relevant to Geological CO_2 Sequestration" is the fourteenth in a series of Geosciences Research Program Symposia dating from 1995. These symposia are topically focused meetings for principal investigators in the program and provide opportunities for our investigators to give presentations on their Office of Basic Energy Sciences' supported research. For this symposium we have developed its program in collaboration with the Environmental Remediation Sciences Division of the Office of Science, the Office of Advanced Scientific Computing Research of the Office of Science and the Regional Carbon Sequestration Partnership Program of the Office of Fossil Energy. I would like to thank them for their contributions. In addition to the recognition the symposium gives to all of the investigators, we traditionally also recognize one outstanding contribution from a DOE Laboratory Project and one from a University Project. The outstanding contributions are selected by our session chairpersons. We are fortunate to have as guest session co-chairs Dr. Dag Nummedal from the Colorado School of Mines, Dr. Robert Burruss from the U.S. Geological Survey, Dr. Rick Allis from the Utah Geological Survey, and Prof. Steven Bryant from the University of Texas at Austin. They join our Principal Investigator co-chairs Prof. Ahkil Datta-Gupta from Texas A&M University, Prof. Art Weglein from the University of Houston, Dr. Ernie Majer of Lawrence Berkeley National Laboratory, and Prof. Laura Pyrak-Nolte from Purdue University. For their efforts on behalf of the investigators I thank them all. We are looking forward to an outstanding series of presentations.

Nicholas B. Woodward
Geosciences Research Program
Office of Basic Energy Sciences
U.S. Department of Energy

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Captions for cover illustrations. Upper image – Processes affecting geologic CO_2 storage and monitoring. Lower left image – Back scatter electron microscopy image of shaley sandstone, with bright K-spar grain along fracture. Lower right image – AVO intercept and gradient profiles for CO_2 injection with t = 10 and 1000 years. Figures courtesy of Sally Benson (Stanford) and Curt Oldenburg (LBNL), Catherine Peters (Princeton), and Ahkil Datta-Gupta (Texas A&M).

Basic Research Relevant to Geological CO_2 Sequestration

-Agenda-

Courtyard Gaithersburg Washingtonian Center

Gaithersburg, MD

March 12-14, 2008

Wednesday, March 12 (AM)

7:30 **Registration/Continental Breakfast**

8:30 **Introductions and Greetings**
Nicholas Woodward, Department of Energy

Session 1

Chairs: Dr. Dag Nummedal (Colorado School of Mines) and Prof. Akhil Datta-Gupta (Texas A&M)

8:45 James Boles, University of California, Santa Barbara
Disequilibrium geochemical signatures in rapidly precipitated $CaCO_3$: Implications for CO_2 sequestration and rates of fault cementation

9:10 David Pollard, Stanford University
Geometric characterization, hydrologic properties, and mechanical behavior of fractures in the analog aquifer/reservoir at the Valley of Fire, Nevada: Implications for CO_2 sequestration

9:35 Russell Detwiler, Lawrence Livermore National Laboratory
Alteration of fracture transmissivities caused by coupled chemical alteration and geomechanical deformation

10:00 Catherine Peters, Princeton University
Upscaling mineral accessibility and pore networks for CO_2 reactive transport in sandstones

10:25 **Coffee/refreshments**

10:50 Harlan Stockman, Sandia National Laboratories
Fingered growth in fractures under flow

11:15 Joel Koplik, City College of New York
Transport and deposition in self-affine fractures

11:40 Peter Eichhubl, Texas Bureau of Economic Geology
Predicting fracture porosity evolution in sandstone

12:05 **Working Lunch**

Wednesday, March 12 (PM)

Session 2

Chairs: Prof. Steven Bryant (UT Austin) and Prof. Arthur Weglein (University of Houston)

1:05 Thomas Dewars, Sandia National Laboratories
Compaction localization, elastic-plastic coupling, and constitutive modeling of Castlegate Sandstone deformation

1:35 Teng-fong Wong, Stony Brook University
Imaging compaction and strain localization in porous sandstone

2:00 Laura Pyrak-Nolte, Purdue University
Effect of a sub-porosity on seismic wave propagation across a fracture

2:25 Amr Abel-Fattah, Los Alamos National Laboratory
Observations of accoustically induced microstreaming and surface clustering of colloidal particles and implications for porous mass transport alteration

2:50 **Coffee/refreshments**

3:10 Karsten Pruess, Lawrence Berkeley National Laboratory
Density-driven brine convection: A process for accelerating CO_2 dissolution and enhancing security of geologic storage

3:35 Roel Snieder, Colorado School of Mines
Monitoring with seismic waves and tilt measurements: Application to Yucca Mountain and fluid transport in the near-surface

4:00 BER/OASCR
Introduction to SciDAC poster presentations

4:20 FE-RCSP
Introduction to Regional Carbon Sequestration Partnership projects and posters

5:00 **Adjourn**

6:00 **Dinner** (On your own)

7:00 RCSP/SciDAC
Poster presentations, Appetizers/Cash bar

Thursday, March 13 (AM)

7:30 **Coffee/Continental Breakfast**

Session 3

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8:20 Nick Woodward
Introduction

8:35 Michael Commer, Lawrence Berkeley National Laboratory
3D fluid imaging using multiple types of geophysical data

9:00 Don Vasco, Lawrence Berkeley National Laboratory
Estimating permeability from quasi-static deformation induced by CO_2 injection: Temporal variations and arrival time inversion

9:25 Gary Egbert, Oregon State University
Computational recipes for electromagnetic inverse problems: Mathematical framework and modular implementation

9:50 Seiji Nakagawa, Lawrence Berkeley National Laboratory
Seismic signatures of fractures and faults: Implications for shear stress monitoring and permeability measurement

10:15 **Coffee/refreshments**

10:35 Akhil Datta-Gupta, Texas A&M University
Time-lapse seismic monitoring of CO_2 sequestration in hydrocarbon reservoirs including compositional and geochemical effects

11:00 Amos Nur, Stanford University
Porous rock with fluids: Applications to CO_2 sequestration

11:25 Jim Berryman, Lawrence Berkeley National Laboratory
Seismic waves in reservoirs with fluids and fractures

11:50 **Lunch** (on your own)

Thursday, March 13 (PM)

Session 4

Chairs: Dr. Robert Burruss (USGS) and Prof. Laura Pyrak-Nolte (Purdue)

1:05 Arthur Weglein, University of Houston
Defining and addressing the pressing seismic exploration and production challenges

1:30 Ilya Tsvankin, Colorado School of Mines
Fracture characterization using prestack amplitude analysis of wide-azimuth seismic reflection data

1:55 Tony Ladd, University of Florida
Pore-scale simulations of erosion in narrow fractures-new methods and applications

2:20 Mack Kennedy, Lawrence Berkeley National Laboratory
Development of isotope techniques for reservoir and aquifer characterization

2:45 **Coffee/refreshments**

3:05 John Morse, Texas A&M University
Reactivity of calcite in saline waters

3:30 Kevin Knauss, Lawrence Berkeley National Laboratory
New experimental approaches to mineral surface chemistry and reactivity characterization

3:55 Daniel Strongin, Temple University
Pyrite surface reactivity under environmentally relevant conditions

4:20 David Cole, Oak Ridge National Laboratory
Rates and mechanisms of mineral-fluid interactions at the nanoscale

4:45 Nick Woodward
Concluding remarks

5:00 **Adjourn**

6:00 **Refreshments**

6:30 **Awards Banquet**

Friday, March 14

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8:10 John Litynski
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9:00 David Wildman
Chapter 3: Geologic characterization

10:00 **Break**

10:20 Bob Finley
Chapter 4: Site development and operations

11:00 David Wildman
Chapter 5: Risk assessment and mitigations strategies

12:00 **Working Lunch**

1:00 Rameshwar Srivastava
Chapter 6: Program implementation

1:45 Sarah Wade
Chapter 7: Public outreach and education

2:30 John Litynski
Chapter 8: Technical transfer

3:00 John Litynski and Nick Woodward
Open discussion and closing remarks

3:30 Adjourn

Disequilibrium geochemical signatures in rapidly precipitated $CaCO_3$: Implications for CO_2 sequestration and rates of fault cementation

James R. Boles[1] and Grant Garven[2]

[1]*Department of Earth Science, University of California, Santa Barbara, CA*
[2]*Department of Geology, Tufts University, Medford, MA*

Carbonate well scales from California oil fields and speleothems in a man-made tunnel show oxygen isotopic disequilibrium, due to CO_2 degassing and *rapid* crystallization. Carbonate growth rates are at mm/year time scales. Most samples are calcite, and some are aragonite or siderite. A few well scales are unusually large crystals of vaterite, an unstable and rare calcite polymorph. The occurrence of aragonite and especially vaterite is mineralogic evidence suggesting rapid disequilibrium crystallization.

The $\delta^{18}O$ of calcites is consistently 1 to 10‰ more positive than expected for equilibrium with pore water. CO_2 degassing preferentially strips the lighter isotopes from the water and leaves precipitated calcite enriched in ^{13}C. Most of the scales have positive $\delta^{13}C$ values (+6.83 to +28.7‰), whereas the speleothems have negative carbon values. All samples show positive $\delta^{13}C/\delta^{18}O$ slopes (typically +0.9 to +5.5), which are intermediate of the proposed range (+0.6 to +8.3) indicative of rapid CO_2 degassing (Hendy, 1971).

Trace element composition of the carbonates can vary widely. Some calcite scales, from waters with constant temperature and fluid composition, show 4 to 16 mole percent Mg content. The relatively constant well bore conditions suggest that precipitation rate may control the Mg content of these scales. Fe substitution is also common in some samples.

Overall these scale and tunnel carbonate samples show the effects of CO_2 degassing and *rapid* crystallization. Comparative studies of carbonates vein-fillings in fault zones do not show this kind of geochemical evidence to support *rapid* crystallization, suggesting that these vein-filling formed at considerably longer time scales than mm/year rates. For example, Garven and his group have used reactive flow modeling methods to quantify effects of fluid mixing and permeability on the geohydrology of mineralization associated with the Refugio Fault, which was constrained by petrologic and geochemical observations from Boles et al. (2004). This model also considers an alternate scenario that hydrocarbons are derived from the deep Eocene strata north of the Refugio fault rather than from the offshore Miocene section in the Santa Barbara channel. This finite element model links evolving fluid chemistry during mass transport and calcite precipitation over time scales of ~5-10 kyrs (Appold et al., 2007).

Geometric characterization, hydrologic properties, and mechanical behavior of fractures in the analog aquifer/reservoir at the Valley of Fire, Nevada: Implications for CO_2 sequestration

Atilla Aydin and David D. Pollard

Department of Geological and Environmental Sciences, Stanford University, Stanford, CA

The Jurassic aeolian Aztec Sandstone in the Valley of Fire State Park, Nevada, provides an exceptional natural laboratory to investigate fluid-fracture interactions in an analog aquifer/reservoir. This presentation is a summary of those investigations that addresses: 1) how various fundamental types of fractures interacted with paleo-fluids; 2) what we have learned about the hydrologic bases for these interactions; and 3) what we have learned about the mechanical behavior of the fractures.

The oldest structures in the sandstone are a result of deformation localization of both shear band and compaction band types. These structures represent significant porosity and permeability reduction with respect to the undeformed rock as determined from image analyses, lattice-Boltzmann flow simulations, and modeling paleo-fluid fronts. The simplest structures are opening mode fractures (joints) that conducted fluids in a fashion close to the idealized parallel plate model with well organized roughness. Sheared-joints which form by slip along pre-existing joints are the simplest shear fractures with slip on the order of millimeters to centimeters. There is abundant evidence that shearing enhanced the conductivity of these fractures by dilation associated with slip across rough surfaces and by linkage through splay fractures. Large-scale shear fractures (faults) are multi-component structures including slip surfaces, fault rocks, and damage zones that are composed of the simpler structures referred to above. Due to this complexity, the interaction between fluids and faults shows a wide range of variation that is demonstrated using observations, lab measurements and up-scaled permeability models.

Inelastic deformation of brittle rock loaded in compression at the meter to kilometer scale typically involves localized frictional sliding along preexisting weak interfaces that are oblique to the principal stress directions. Associated local stress concentrations can produce secondary opening fractures in the fault damage zone that emanate from the sides of faults as wing cracks. The formation of wing cracks is closely related to important geological phenomena observed in the Aztec Sandstone such as propagation of shear fractures, fault coalescence and longitudinal growth, the formation of fault damage zones, and fluid flow channeling. The 2D Displacement Discontinuity Method (DDM) is combined with a complementarity algorithm to model the quasi-static formation and patterns of wing cracks that emanate from regions of stress concentration along a sliding frictional flaw in an otherwise homogeneous and isotropic elastic material.

We conclude that the Valley of Fire analog aquifer/reservoir displays excellent examples of fluid-fracture interactions with a wide diversity, controlled primarily by the failure modes, and that flow and mechanical modeling at various scales reveals the fundamental physical processes responsible for the nature of the observed interactions.

Alteration of fracture transmissivities caused by coupled chemical alteration and geomechanical deformation

Russell Detwiler

Lawrence Livermore National Laboratory, Livermore, CA

Flow through fractures is controlled by the magnitude and variability of apertures within the fracture. Geochemical reactions and applied stresses can alter fracture apertures leading to changes in transmissivity that are difficult to predict with existing models. Previous experimental studies in fixed displacement fractures have shown that flow of reactive fluids can lead to different dissolution patterns that are controlled by the Peclet (Pe ~ advection/diffusion) and Damkohler (Da ~ reaction/advection) numbers and range from development of distinct channels (low Pe, high Da) to relatively uniform dissolution throughout the fracture (high Pe, low Da). Under conditions favoring more uniform dissolution the smallest aperture regions dissolve more quickly than the larger apertures, leading to a smoothing of the fracture aperture field. This suggests that, under certain conditions, the addition of normal stresses, which can be significant in many subsurface environments, may lead to closure of the fracture surfaces and reduced transmissivity (*T*).

We have developed an experimental system that allows application of a steady confining stress to transparent analog, variable-aperture fractures during reactive fluid flow experiments. The fractures are fabricated by mating a rough, nonreactive surface (glass) with a smooth reactive surface KH_2PO_4. We present results from two experiments in identical fractures in which the flow rates (and hence *Da*) differed by a factor of two Because the fractures are transparent, we can apply light transmission techniques to accurately (± 6 μm) measure fracture apertures at high spatial resolution (80 x 80 μm) over the entire flow field during dissolution experiments. In addition, LVDTs measure relative displacement of the fracture surfaces during experiments. At early time, surface dissolution led to gradual increases in fracture transmissivity with rates roughly proportional to the flow rates; and negligible displacements of the surfaces suggested the absence of pressure-enhanced dissolution of contacting asperities. After this initial phase, disparate behavior was observed in the two experiments: (1) During the high-flow-rate experiment (lower *Da*), more uniform dissolution caused simultaneous erosion of numerous contacting asperities leading to larger stresses and eventual failure of the asperities. This resulted in large (20-50 μm) instantaneous displacements, which occurred periodically during the experiment, followed by periods of approximately constant-rate steady displacements. The overall effect was that after the initial period of increasing transmissivity, the periodic oscillations caused by surface displacements competing with surface dissolution, led to a gradual decline in *T*. (2) During the low-flow-rate experiment, (higher *Da*) the instantaneous displacements due to failure of asperities were much smaller due to the formation of a large-scale channel that left regions of the fracture relatively unaffected by dissolution. Thus, in this experiment, the initial period of steadily increasing *T* continued despite small surface displacements because the rate of surface dissolution exceeded the rate of fracture closure.

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Upscaling mineral accessibility and pore networks for CO_2 reactive transport in sandstones

Catherine A. Peters[1], W. Brent Lindquist[2], and Michael A. Celia[1]

[1]*Civil and Environmental Engineering, Princeton University, Princeton, NJ*
[2]*Applied Mathematics and Statistics, Stony Brook University, Stony Brook, NY*

Widespread implementation of geological storage of CO_2 will require an understanding of acid-driven reactions with formation minerals. Predicting these reactions and their time scales requires rate laws that are appropriate for sedimentary rocks and estimates of accessible surface areas of reactive minerals. This project addresses these needs through a study that combines imaging of sandstone pore structure and minerals, and network-modeling of reaction rates in porous media. Rock specimens come from the Viking formation in the Alberta Sedimentary Basin. Imaging methods include X-ray computed microtomography (CT), backscatter electron microscopy (BSE) and energy dispersive X-ray (EDX) spectroscopy.

One important goal is to characterize pore contact with individual minerals thereby quantifying meaningful surface areas for use in reactive transport models. The suite of techniques employed and the innovative means by which the images are collectively interpreted provides a wealth of information to address this goal. For example, a novel method of interpreting BSE images (which are high resolution) combined with EDX images (which can generate mineral maps) leads to 2D images that provide detailed characterization of the proximity of reactive minerals to pore space. Extension of this image processing approach to 3D, using CT images to broadly classify mineral categories, allows us to relate detailed information about pore structure with mineral accessibility, albeit with coarser resolution.

All the specimens are sandstones of comparable porosity and grain diameter, and yet order of magnitude variation is found in pore structure and reactive mineral properties across them. In general, we have found that mineral volumetric content is a poor indicator of proportionate pore-to-mineral surface area due to the means by which minerals are obscured in consolidated media. For example, kaolinite and other authigenic clay minerals that coat grains and fill primary pore space account for only 5% to 30% of mineral content, but 65% to 90% of pore-mineral contact boundaries. Minerals that would react under acidic conditions may account for 5% to 10% (vol.) of mineral matter, but if these percentages are used to apportion surface area, they would overestimate reaction rates by three to five times.

These detailed characterizations of pore structure and mineral spatial patterning are being used to develop pore-network models that simulate reactive transport. Simulations of conditions representative of CO_2 injection for geological storage are being used to examine up-scaling of reaction rates from the pore-scale to the core-scale.

Fingered growth in fractures under flow

Harlan W. Stockman

Sandia National Laboratories, Las Vegas, NV

Upstream fingered or dendritic growth is a well-established form of solids precipitation. Such growth could lead to rapid closure of fractures and radical decreases in permeability, after just a small fraction of the fracture volume is filled. Newhouse (1941) argued that the direction of solids growth in ore samples could be used to infer the direction of aqueous flow; his argument, with some qualification, is that the solutions initially encounter the upstream side of the growing solid, thus first precipitate material on the upstream side. Thus growing crystals will point into the flow. However, it is unclear if such growth would occur in geological conditions, even under the extreme oversaturation encountered in waste disposal sites. Experimental observation of fingered- and flow-affected growth has typically been limited to rapid crystallization of non-faceting single crystals.

This study attempts to determine if such directional growth would be observable in laboratory experiments performed with slower-growing, multicrystalline solids. The hypothetical laboratory experiments involve flow of 1 mm/s through transparent Hele-Shaw cells separated by 1 mm. The modeling is performed by 3D lattice-Bolzmann (LB) with kinetic precipitation and dissolution algorithms.

Initial LB calculations suggest there is a fairly limited set of conditions where the proposed behavior actually occurs; the solubility of the solid must be high, yet the precipitation rate must be fast, and flow must be uncomplicated enough to prevent vortices from mixing the solutes. The fingering or dendritic growth is discernable best at high diffusive Dahmkoler number ($Da > 10^4$), and the results are most apparent from a statistical analysis of many realizations, as very slight variations in initial conditions dramatically change the pattern of dendrite growth at high Da. Even then the “fracture” surfaces must be highly regular; else one simply sees growth toward the highest flow speed, which is often a channel not coincident with the bulk flow. The precipitates at high Da tend to be porous, with long fingers that effectively stop local flow, yet fill less than 30% of the available space. The precipitates at low Da (25 or less) are more compact and non-fingered, but still show a smaller, statistically discernable tendency to grow on the upstream side. However, this measurement of growth is possible because the initial location of the seed is known exactly in the LB simulations; such information might not be available in geologic settings. Most geological precipitates are expected to be typical of lower Da conditions, so fingered and directional growth (observable in fractures) may actually be an anomaly. Simulations of seeded growth with polycrystalline gypsum indicate that the enhanced and directional growth would be subtle. Flow does enhance the total deposition rate of solid materials, by stripping away the diffusive boundary layer that would occur in static environments. However, this enhancement also becomes much less apparent as the Da decreases.

Newhouse, W.H. (1941) The direction of flow of mineralizing solutions. ***Econ. Geol.*** **36**, 612-629.

Transport and deposition in self-affine fractures

Joel Koplik

Levich Institute, City College of New York, New York, NY

Geological fracture surfaces have a correlated roughness which can be quantified as "self-affine fractal," meaning that the correlation function of the surface fluctuations at different points varies as a power of the distance between them. The power in question is called the Hurst exponent, and is somewhat universal with only two typical values observed. This project studies the consequences of fractal roughness on the transport of fluids and particles in self-affine fractures, and in this presentation we discuss two recent developments.

(1) The fluid present in fracture systems often has non-Newtonian rheology, the simplest example of which is a power-law dependence of viscosity on strain rate. We have developed a lattice-Boltzmann computational method to calculate such flows, and used it to examine the variation of permeability with Reynolds number, power-law exponent and Hurst exponent. The results are very analogous to the behavior of Newtonian fluids in rough pipes and both Newtonian and non-Newtonian fluids in inter-granular porous media, and can be quantified in a universal plot of friction factor vs. Reynolds number.

(2) The fluids present in fracture systems relevant to aquifers and hydrocarbon reservoirs also often contain particulates of various sizes, and we have used lattice-Boltzmann to study pressure driven flow and deposition of suspensions through flat-walled and self-affine channels. The behavior of a suspension is controlled by the buoyancy number, the Reynolds number and the initial particle concentration, and typically evolves into three spatial domains - a deposition region, a suspension region, and a clear region. The range of the three domains is predominantly controlled by the buoyancy number, while the particle flux and deposit packing is largely related to the Reynolds number. We observe surface particle transport atop deposited layers, which is related to the shear stress along the surface of the deposition bed. We relate the microstructure of the suspension and deposition to those macroscopic transport properties.

Predicting fracture porosity evolution in sandstone

Stephen E. Laubach[1], Peter Eichhubl[1], Robert H. Lander[2], Jon E. Olson[3], Linda M. Bonnell[2], Julia Gale[1], Randall Marrett[4]

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[4] *Department of Geological Sciences, The University of Texas at Austin, Austin TX*

Fluid flow in fractured rock is an increasingly central issue in recovering water and hydrocarbon supplies and geothermal energy and in predicting subsurface movement of pollutants, including anthropogenic CO_2. Yet mechanical models typically neglect cementation in fractures and the rock mass, tacitly assuming that cementation rates are slow relative to fracturing and that fracture growth and fracture filling are decoupled. We investigate how fracture growth and diagenetic alteration interact to create and destroy fracture porosity in sandstone reservoirs. We are testing the hypothesis that records of fracture opening can be recovered from fractures formed in the subsurface and that, along with fluid-inclusion data and diagenetic and geomechanical models, these records can help recover duration and rates at which fractures open and rock properties change.

We apply large-area (mm^2) cathodoluminescence (CL) imaging and mapping methods and fluid-inclusion analysis and crystallographic analysis using electron backscatter diffraction methods of partly sealed fractures to reconstruct sequential trapping of fluid inclusions during fracture opening. Synkinematic cement bridges are a common fracture attribute in moderately to deeply buried rocks (1+-km depth). We reconstruct fracture-opening history from CL image maps and fluid inclusions trapped within individual cement layers defined by crack-seal texture. In core and outcrop examples, any single bridge may contain many tens to hundreds of generations of fluid-inclusion assemblages (FIAs) that record thermal and chemical characteristics of fluids present during crack-seal events. Analysis of these FIAs across the fracture reveals the history of temperature change; high-resolution CL imaging defines relative ages of FIAs. With a burial history, fracture age is obtained by comparing time-temperature curves. Reconstructions of fracture-aperture development tied to burial-history analysis indicate that fractures grow episodically during as much as tens of millions of years. Geomechanical models incorporating diagenesis produce fracture size and spatial arrangement patterns that cannot be accounted for when diagenesis or mechanics are treated as separate, isolated processes.

Compaction localization, elastic-plastic coupling, and constitutive modeling of Castlegate Sandstone deformation

Thomas Dewers[1], Kathleen Issen[2], David Holcomb[1] and William Olsson[1]

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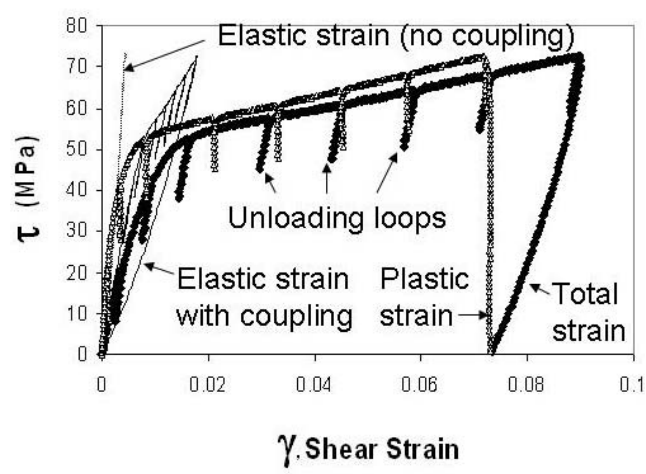
[2]*Clarkson University, Wallace H. Coulter School of Engineering, Potsdam, NY*

Castlegate Sandstone is a weak porous rock often invoked as a reservoir analogue. Work by Olsson (1999) and Holcomb and Olsson (2003) demonstrate that Castlegate exhibits localized compactive behavior with attendant order of magnitude changes in permeability. *In situ* this behavior would significantly change the ability to extract and inject fluids into reservoirs. A series of axisymmetric compression tests were performed at a variety of mean stresses to study a range of expected behaviors, including dilational (brittle, low mean stress), compactional (ductile, high mean stress), and transitional, with attention paid to variations in localization behavior in dilational and transitional regimes. In most tests, unloading-reloading loops were performed tracking evolution of elastic properties with progressive plastic straining. The goal was to derive a complete set of constitutive parameters suitable for use in testing the applicability of theories of localization, both shear and compactive, to porous reservoir sandstones.

Isotropic bulk and shear moduli are found to evolve as increasing functions of mean stress σ and Mises equivalent shear stress τ respectively, and as decreasing functions of work-conjugate inelastic strains. This permits a partitioning of elastic and plastic strains during the tests. With σ_{ij} and C_{ijkl} as stress and compliance tensors, total strain increments are divisible into four parts, i.e., $\dot{\varepsilon}_{ij} = \dot{\varepsilon}^1_{ij} + \dot{\varepsilon}^2_{ij} + \dot{\varepsilon}^3_{ij} + \dot{\varepsilon}^4_{ij}$ where $\dot{\varepsilon}^1_{ij} = C_{ijkl}\dot{\sigma}_{kl}$ (constant moduli), $\dot{\varepsilon}^2_{ij} = \dfrac{\partial C_{ijkl}}{\partial \sigma_{mn}}\sigma_{kl}\dot{\sigma}_{mn}$ (increase in moduli with stress as a result of crack closure etc.), $\dot{\varepsilon}^3_{ij} = \dfrac{\partial C_{ijkl}}{\partial \varepsilon^p_{mn}}\sigma_{kl}\dot{\varepsilon}^p_{mn}$ (modulus degradation with plastic strain) and $\dot{\varepsilon}^4_{ij} = \dot{\varepsilon}^p_{ij}$ (plastic strain). In this sense 1- 3 are "elastic", 4 is plastic, 1 & 2 are reversible, and 3 & 4 are irreversible. The term labeled 3 is the elastic-plastic coupling strain increment, and though often ignored, can be a large contributor to the total strain, particularly for brittle and transitional tests pre-failure. An example of strain partitioning for a high mean stress (σ = 150 MPa) test is shown graphically in the figure at left.



Plastic strains are commonly calculated by subtracting terms 1 and 2 from the total strain. We refer to this as the uncoupled case. If the contribution of the modulus degradation is also subtracted then the result is the coupled plastic strain. Plastic strain calculated with and without the coupling term (3) can be compared with regard to localization predictions. Using the Rudnicki and Rice (1975) formulation as adapted by Issen and Rudnicki (2000; 2001) for compaction localization, both coupled and uncoupled cases predict high angle shear bands for uniaxial and low mean stress tests well on the dilational side of the yield surface. Uncoupled predictions show progressively lower angle shear bands approaching the transitional regime (approaching the "cap" surface). When elastic-plastic coupling is accounted for, compaction bands are predicted for the transitional regime, as are observed in the Castlegate tests. This is the first time that localization calculations have been successful in predicting compaction bands using the Rudnicki and Rice treatment, suggesting an important role of coupling strains in constitutive models for weak sandstones.

Lastly, we briefly describe modeling efforts using Sandia's Geomodel (Fossum and Brannon, 2004), a 3-invariant, mixed-hardening, continuous yield surface, elasto- plasticity model that includes several features important in modeling Castlegate Sandstone constitutive behavior, including non-associativity, nonlinear elasticity, elastic-plastic coupling, and kinematic hardening.

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Imaging compaction and strain localization in porous sandstone

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Strain localization develops over a broad range of length scales, and it is a deformation and failure phenomenon which is accompanied by dilatancy or compaction. The damage evolution associated with such dilatant or compactant failure can potentially be imaged nondestructively by X-ray computer tomography (CT). Whereas a dilating shear band is relatively easy to image because localized dilatancy is very effective in enhancing the contrast in X-ray attenuation between the band and its surrounding, corresponding contrast due to localized compaction is appreciably less. In this pilot study, we tackled this challenge in imaging compaction and strain localization by testing the feasibility of two techniques in porous sandstone. CT images of the sandstone samples were acquired at the High-Resolution CT Facility at UT Austin.

In the first approach, we developed a statistical technique for mapping out the spatial distribution of compactant cataclastic damage due to grain crushing and pore collapse. Our data demonstrate that such micromechanical processes would appreciably decrease both the skewness and dispersion of CT-values of an ensemble of voxels. Using the coefficient of variation for 27 voxels embedded in a cube with volume comparable to that of a grain, we were able to obtain a local measure of damage which maps out the 3D geometric complexity of discrete compaction bands developed in a compacted sample of Diemelstadt sandstone. Our interpretation of the CT data was validated by microstructural observations, which also provide constraints on the binarization of CT images for quantitative characterization of the width, tortuosity and orientation of discrete compaction bands and for inference of permeability evolution.

In the second approach, X-ray radiographs were acquired before and after a deformation experiment, and 2-D digital image correlation (DIC) was performed to map out the spatial distribution of compactive strain in the failed sample. We also investigated the effect of the bedding on the development of strain localization in Rothbach sandstone. Our technique could resolve the spatial distribution of strains on the order of 10^{-3}, and DIC of CT images of three sandstone samples cored in three orientations underscore different modes of localization. While diffuse compaction bands and compactive shear bands developed in the samples perpendicular and oblique to bedding, relatively homogenous compaction was observed in the sample cored parallel to bedding. The strain patterns inferred from DIC were confirmed by complementary microstructural study including quantitative characterization of crack density.

This pilot study has demonstrated the potential of extending the statistical and DIC techniques to higher resolutions using synchrotron microCT data of triaxially compressed rock samples.

Effect of a sub-porosity on seismic wave propagation across a fracture

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Fractures and joints in the field often contain debris within the void spaces (aperture). These debris originate from many different mechanisms: organic and/or inorganic chemical reactions (such as mineralization), sediment transport, formation of the fracture, mechanical weathering, or combinations of these processes. In many cases, the debris forms a "sub-porosity" within the fracture void space. This sub-porosity often is composed of material that differs from or can be the same as that of the fracture walls in chemical and physical composition. The "sub-porosity" may partially fill the fracture void space, thereby reducing the local porosity, or sometimes can fill completely the void spaces, in either case affecting the hydrologic properties of the fracture, such as fracture porosity, permeability and storativity. In this study, we investigate how a sub-porosity affects seismic wave propagation across the fracture, and we test the ability to probe changes in the fracture properties caused by the formation or alteration of a sub-porosity.

Laboratory experiments were performed to examine seismic wave scattering from packings of particles that create a sub-porosity within a synthetic fracture. Sub-porosities were created in four manners: (1) from spherical beads (acrylic, soda-lime glass or borosilicate materials) with a range of diameters from 25 μm to 7.79 mm; (2) from 100 micron to 200 microns particles of metallic salts; (3) from 750 micron to 850 microns particles of $C_3H_3NaO_2$ (Poly Acrylic Acid Sodium Salt); and (4) biomimetic growth of fluoro-apatite spheres. Compressional and shear waves were transmitted across the fracture using contact piezoelectric transducers (central frequency 1 MHz) for a fixed aperture size filled with the different sub-porosity packings. A time-frequency analysis was performed to obtain the dispersion of waves transmitted across the fracture partially filled with debris.

The ability to distinguish a partially particle-filled fracture from an open fracture (all water-saturated) depends on the size of the sediment grains relative to a wavelength as well as on the material that composes the sub-porosity. In this study we observe that dispersion, interference nulls and wave speed are the prime indicators of the presence of a sub-porosity created by particles within a fracture, and that shear waves are particularly sensitive to the cohesiveness of the particles composing the sub-porosity. These results open the possibility for active monitoring of fracture alterations using shear waves to sense saturated fracture subporosity changes, while using compressional waves as a normalization standard.

Observations of acoustically induced microstreaming and surface clustering of colloidal particles and implications for porous mass transport alteration

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Elastic waves are known to induce observable changes in porous mass transport behavior in the Earth and geomaterials. Reported observations of this “Dynamic-Stress-Stimulated Transport” (DSST) phenomenon include oil reservoir production increases induced by seismic (1 to 500 Hz) waves and permeability enhancement in sandstone by ultrasonic (10 to 100 kHz) energy. Potential applications include accelerated contaminant extraction from groundwater aquifers, controlling subsurface transport at waste containment facilities and manipulating formation permeability for improved CO_2 sequestration. Our ongoing OBES project is focused on understanding elastic-wave coupling to colloid interactions in aqueous systems. These interactions play a major role in DSST phenomenon because the distribution of solid colloids in a porous medium can directly affect its permeability and fluid transport properties, possibly over large distances. Thus, it is important to understand the fundamental interaction mechanisms because colloid mobility at the pore scale (μm) can have profound effects on porous media permeability at the core (cm to m) and field (m to km) scales. Two unique experimental laboratory facilities developed at LANL are being used to study elastic-wave influences on colloid behavior at both microscopic and core scales.

Microscopic visualization experiments were performed to study acoustically-induced colloid behavior at relatively high frequencies (200-500 kHz) and different ionic strengths. Green fluorescent (468/508 nm wavelength) polystyrene microspheres with a mean diameter of 2.26-μm and density of 1.05 g/cm^3, were suspended in either deionized water or a 0.1*M* NaCl solution and injected into a parallel-plate glass flow cell. Acoustic stimulation of the cell at 313 kHz induced three distinct particle behaviors: 1) entrainment and bulk transport via wavelength-scale Rayleigh streaming, 2) entrapment via boundary layer vorticular (Schlichting) microstreaming, and 3) chain-like clustering at the higher ionic strength. These three types of behavior represent important physical mechanisms whereby acoustic energy is capable of affecting colloid mobility and distribution. Colloid trapping at pore walls or formation of aggregates at pore throats will reduce the matrix permeability. Colloid release from pore walls or breakup of aggregates plugging pore throats will increase the permeability. These micro-scale acoustic effects, however, are strongly coupled with electrokinetic effects. The experiments showed that it is extremely difficult to detach particles from solid surfaces or break up aggregates with acoustics alone when the suspending fluid has a relatively high ionic strength. This result implies that near-surface boundary layer forces that are known to be altered by electrokinetic phenomena (streaming potential and electrophoresis) are too strong for acoustically induced hydrodynamic forces to overcome.

Effects of dynamic stress on core-scale (cm to m) bulk-fluid porous flow are being investigated in the seismic range of frequencies (1-500 Hz) using a core-flow apparatus that mechanically strains 2.54-cm-diameter porous rock samples during constant-rate fluid flow. Numerous experiments were performed to study the ability of low-frequency (1-500 Hz) dynamic stress to mobilize colloids trapped in a Fontainebleau sandstone core. Of major relevance are those involving 1) natural *in situ* colloid production, and 2) injection and transport of synthetic microspheres. Cumulative results of the core transport experiments indicate that low-frequency stress waves can mobilize colloids and increase permeability when the particle-trapping mechanism does not involve colloidal forces. Low ionic strength is required to detach colloids from pore walls. Colloid fouling of pore throats can be broken up by dynamic stress only if hydrodynamic forces alone cause the bridging, which only occurs at low ionic strength. Thus, the low-frequency, core-scale behavior agrees qualitatively with the high-frequency micro-scale behavior.

Density-driven brine convection: A process for accelerating CO_2 dissolution and enhancing security of geologic storage

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For purposes of geologic storage, CO_2 would be injected into saline formations at supercritical temperature and pressure conditions, and would form a separate phase that is immiscible with the aqueous phase (brine). Supercritical CO_2 ($scCO_2$) has lower density than the aqueous phase and would experience an upward buoyancy force, rising to the top of the permeable formation, and spreading out laterally beneath a low-permeability caprock. Free CO_2 is highly mobile due to its low, gas-like viscosity, and could escape from the storage formation wherever (sub-)vertical pathways are available, such as fractures or faults through the caprock, or improperly abandoned wells. Over time, an increasing fraction of CO_2 may dissolve in the aqueous phase, and eventually some of the aqueous CO_2 may react with rock minerals to form poorly soluble carbonates. Dissolution into the aqueous phase and eventual sequestration as carbonates are highly desirable processes as they would increase permanence and security of storage. If the aqueous phase were immobile, CO_2 dissolution would be limited by the rate at which aqueous CO_2 is removed from the interface between CO_2-rich and aqueous phases by molecular diffusion in the aqueous phase. This is a very slow process. However, dissolution of CO_2 is accompanied by a small increase in the density of the aqueous phase, creating a negative buoyancy force that could give rise to downward convection of CO_2-rich brine, greatly accelerating the dissolution of the free CO_2.

The buoyant convection process induced by denser aqueous phase overlying less dense fluid is intrinsically multi-scale in nature, i.e., at early time the process occurs on the scale of a few pores and over time grows by many orders of magnitude to eventually encompass field-scale convection and mixing. The objectives of this project are to study and visualize the process of dissolution-diffusion-convection (DDC) through laboratory experiments, and to develop multiscale numerical techniques for representing DDC in coarsely-gridded field scale problems.

This project has just started and the presentation will summarize current understanding and preliminary results.

Monitoring with seismic waves and tilt measurements; Application to Yucca Mountain and fluid transport in the near-surface

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We present a progress report of research in two novel techniques for remotely monitoring the sub-surface. The 1997-2002 Yucca Mt. heated drift experiment used a specialized system of heaters to simulate stored nuclear waste and effects of radioactive decay heating on the tunnel, surrounding rock, and groundwater flow. While calibration shots were recorded on a seismic array installed around the tunnel, wall temperatures were elevated to 200-degrees Centigrade. Receiver gathers show classic wave propagation behavior as verified in the literature for pulses incident upon cylinders (the tunnel). The addition of heat, and resulting groundwater dry-out causes changes in direct and reflected P-S waves that propagate in the surrounding tuff. Data also show that the same waveforms effectively do not change once the target temperature is obtained at the tunnel wall. 2-D waveform simulation coupled with well-constrained thermal models has consistently replicated receiver data in the plane of the calibration source. Analytical and experimental work has also shown the presence of a "Franz" wave propagating perpendicular to the tunnel wall at low velocities. This wave is also present in field and model data at speeds that vary with thermal input. P-S wave separation and Franz wave velocity are potential tools for seismically measuring the diameter of groundwater saturation around the tunnel. Lack of change in the waveforms occurring for constant temperature infers material change has ceased in the rock matrix and groundwater processes no longer effect wave speed

We carried out a field experiment in Arizona where a field was irrigated twice; once with water and once with a surfactant. The site was extensively instrumented, and we analyze the tilt-measurements in three boreholes. The tilt measurements are dominated by transient signals associated with earthquakes, human activity, and settling of the instruments. Careful processing of the tilt data allowed us to extract the tidal response from these data. A preliminary analysis shows that the 12h tidal response changes during the irrigation with the surfactant. Back of the envelope calculations show that a perturbation of the elastic parameters in the irrigated area of a few percent should leave a measurable imprint on the tilt measurement. Current work focuses on analyzing longer time series, and on a quantitative interpretation of the perturbations in the tidal response.

3D fluid imaging using multiple types of geophysical data

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Large-scale 3D geophysical imaging is now receiving considerable attention for electrical conductivity mapping of fluids associated with potential energy resources (fossil and geothermal). The technology also has direct relevance to monitoring sequestration of CO_2 fluids with time lapse imaging experiments. Because of the large computational requirements of the 3D imaging problem, new strategies that exploit computational parallelism and optimized finite-difference meshing have been developed and successfully demonstrated on industrial size field data sets and we will report on several experiments. However, we now believe that we will soon reach the point where further improvement in subsurface 3D image reconstruction will require multiple types of geophysical data measurements. For example, 3D conductivity imaging using magnetotellurics (MT) and controlled source electromagnetic (CSEM) data sets has much appeal and when combined should provide superior imaging, than can be obtained using CSEM or MT data sets in isolation. There is clear evidence that CSEM methods are more sensitive to fluid identification in geological bedding, including brines, hydrocarbons and possibly CO_2. MT methods on the other hand provide valuable information on controlling geological structures where fluids are found. Moreover there are overlaps in the measurement acquisition of these methods leading to efficiencies and reduced costs when the data are acquired jointly. Joint imaging of EM and seismic data also has much appeal, and may yield an optimal imaging technology for fluid identification and transport properties of the subsurface (porosity, saturation and permeability). These properties are often times of much greater interest than the geophysical parameters. In this talk we will report on our ongoing and planned research efforts on these topics.

Estimating permeability from quasi-static deformation induced by CO_2 injection: Temporal variations and arrival time inversion

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Transient pressure variations due to CO_2 injection within a reservoir can be treated as a propagating front and analyzed using an asymptotic formulation. From this perspective one can define a pressure 'arrival time' and formulate solutions along trajectories, in the manner of ray theory. I combined this methodology and a technique for mapping overburden deformation into reservoir volume change as a means to estimate reservoir flow properties, such as permeability. Given the entire 'travel time' or phase field, obtained from the deformation data, I constructed the trajectories directly, thereby linearizing the inverse problem. A numerical study indicated that, using this approach, one may infer large-scale variations in flow properties. In an application to Interferometric Synthetic Aperture (InSAR) observations (Figure 1, left panel) associated with a CO_2 injection in well KB501 at the Krechba field, Algeria, I imaged pressure propagation to the northwest. An inversion for flow properties indicated a linear trend of high permeability (Figure 1, right panel). The high permeability correlated with a northwest trending fault on the flank of the anticline defining the field.

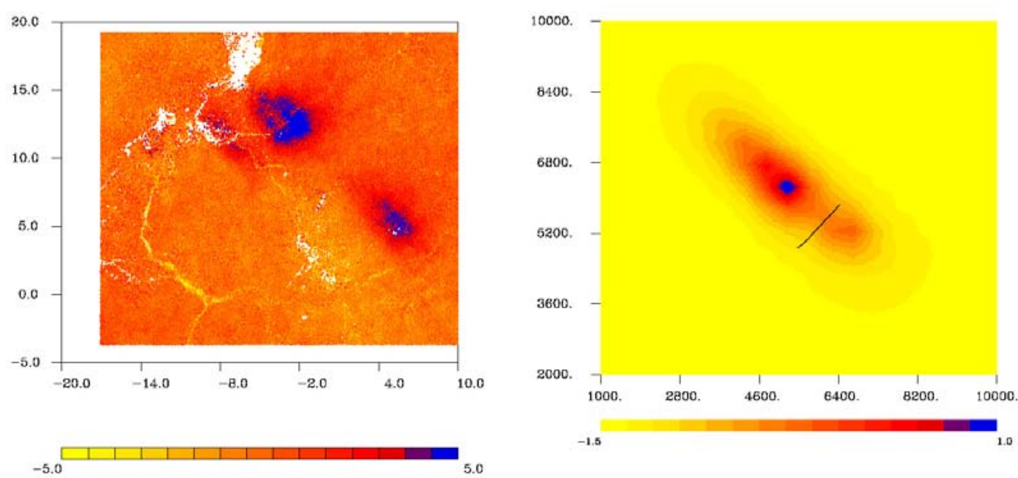

Figure 1

Another application to Interferometric Synthetic Aperture Radar (InSAR) data gathered over a CO_2 injection at well KB502 at the Krechba field reveals pressure propagation along two northwest trending corridors. Changes outside the boundaries of the 20 m thick reservoir are required to produce a plausible distribution of pressure variations. Two northwest trending high permeability zones are imaged, trending in the same direction as the regional fault and fracture zones.

Computational recipes for electromagnetic inverse problems: mathematical framework and modular implementation

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Three-dimensional inversion of electromagnetic (EM) data for subsurface imaging presents a number of challenges. The forward problem for EM imaging is computationally demanding, requiring numerical solution of a system of partial differential equations for each source configuration. For typical applications there are multiple transmitters (different frequencies and/or locations), so many numerical solver calls are required even for the forward problem. Even more complex and demanding multi-transmitter computations are needed for computation of data sensitivities, or of penalty functional gradients. Thus, 3D EM inversion results in very large computational problems that do not scale well as the number of available data and the spatial resolution required for realistic 3D imaging applications increases. At the same time, development of practical and capable computer codes for EM inversion is a complex enough task that interpretation tools have lagged recent advances in data acquisition technology. In our presentation we provide an overview of our recent efforts to help overcome some of these challenges. Our approach has been to first formalize and abstract common algorithms used for gradient-based inversion of EM data, and then, based on this formalism, develop general computational recipes and modular computer codes for a broad class of EM inverse problems. The general formalism suggests computational efficiencies including (1) hybrid inversion algorithms, which combine elements of an iterative conjugate gradient scheme with a Gauss-Newton type Occam scheme, based on computation of the full Jacobian (matrix of partial derivatives) of the model parameter-data mapping; (2) ways to take advantage of the special structure of the Jacobian in multi-transmitter EM problems to develop more efficient computational strategies; and (3) approximate highly efficient schemes for multi-frequency problems. We will also discuss development of a modular system of computer codes that we are developing for general EM inverse problems. The modular system allows rapid prototyping and testing of the proposed new algorithms. In particular, the system allows initial testing and debugging on simpler 2D problems, followed by relatively seamless transition to more computationally demanding 3D problems. The modular system allows substantial code reuse on different problems, extensibility (e.g., adding new data types, observing system configurations, or model parameterization/regularization), and maintenance/upgrading of code (e.g., incorporating more efficient or accurate forward solvers). Example applications will be taken from 2D and 3D finite difference implementations for magnetotelluric and controlled source EM problems.

Seismic signatures of fractures and faults: Implications for shear stress monitoring and permeability measurement

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Fractures and faults define important permeability boundaries (both sealing and conducting) that dominate subsurface fluid migration. For successful geological CO_2 sequestration, accurate knowledge of these boundaries is essential for predicting the movement of the injected fluid. Also, during extraction and injection of fluids in a reservoir, these boundaries can be activated in response to changes in shear stress, potentially resulting in a breach of the seal rock. Thus, seismic monitoring of the shear stress on fractures and faults is desirable—and maybe even possible (Nakagawa et al., 2000). The main objectives of this research are: (1) to understand how shear stress effects previously discovered unconventional seismic-wave mode conversion (scattering of normal-incidence compressional waves to shear waves, and vice versa); (2) to establish simple models for studying poroelastic properties of a fluid-bearing fracture; and (3) to examine the effect of fracture and fluid properties—such as fracture compliance, permeability, and fluid viscosity—on the scattering of seismic waves.

We conducted a series of laboratory experiments to examine how the relative magnitude of normal and shear stresses on a fracture and the loading history of the shear stress affect the amplitude of shear-stress-induced seismic wave mode conversion. The results showed that the amplitude of the converted wave increases linearly with applied shear stress for small shear stresses, but that the amplitude increase is less for higher shear stresses (nonlinear response). The experiment also indicated that the conversion can result from both elastic deformation and inelastic slip of the fracture surface.

Next, for examining the seismic properties of a fluid-bearing fracture, we expanded a simple theoretical model for a (visco) elastic fracture (commonly called *seismic displacement-discontinuity model* or *linear slip interface model*) to a poroelastic fracture. This modeling was conducted by envisioning a compliant fracture as a thin, flat, homogeneous poroelastic layer, resulting in matrix boundary conditions that define a new set of characteristic fracture parameters (analogous to fracture stiffness and compliance). Interestingly, numerical simulations using the model indicated that, for a thin fracture, the fracture-parallel permeability did not affect seismic wave scattering.

We suspected that the cause of this counterintuitive result was the lack of fracture heterogeneity in the model. Focusing on a partially open, permeable fracture, we examined the effect of fracture heterogeneity on seismic wave scattering—including fracture compliance, fracture opening (defined through the hydraulic properties of a fracture), fluid properties (including saturation ratio), and fracture-parallel flow permeability. For this purpose, the original poroelastic fracture model was first revised to include the effect of local fluid flow in the fracture. Subsequently, using this model, we developed a plane-wave method to compute the scattering of incoming waves by a fracture with arbitrary distributions of fracture characteristic parameters. Computational results using this method showed that heterogeneity in fracture compliance and fracture width alone still does not make the scattering of seismic waves permeability dependent. However, a very small amount of gas within the fracture was found to cause a significant effect on wave scattering, which is now a function of fracture permeability.

Time lapse seismic monitoring of CO_2 sequestration in hydrocarbon reservoirs including compositional and geochemical effects

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We examine the viability of time-lapse seismic monitoring using an integrated modeling of fluid flow, including compositional and geochemical processes, and seismic response. Modeling of CO_2 injection is complicated by the various interactions between CO_2, reservoir fluids and the minerals in the formation. These interactions change fluid and bulk rock properties with time, which in turn impact the seismic signatures. In particular, for modeling and performance assessment of large-scale CO_2 sequestration projects, we need efficient approaches for numerical simulation of compositional and geochemical processes in the reservoir.

We have developed a streamline-based compositional transport model for CO_2 injection that can be orders of magnitude faster than conventional finite-difference models. Our compositional streamline formulation, for the first time, rigorously accounts for compressibility effects by introducing the concept of 'effective density' to redefine the bi-streamfunctions and decouple the 3D conservation equations to 1D transport equations for overall compositions along streamlines. The 'effective density' accounts for volume changes with pressure and can be conveniently traced along streamlines. The streamline equations are solved using a third order total variation diminishing (TVD) scheme to minimize numerical dispersion. The phase compositions and saturations are obtained via thermodynamic flash calculations.

We perform a comprehensive simulation of the gas injection process accounting for the phase behavior of CO_2-reservoir fluids, the associated precipitation/dissolution reactions and the accompanying changes in porosity and permeability. The simulation results are then used to model the changes in seismic response with time. The general observation is that gas injection decreases bulk density and wave velocity of the host rock system. Seismic amplitude attributes therefore change with time as well, and these effects provide a tool for tracking the movement of the CO_2 front. Analysis of the results also confirms that much of the change can be attributed to chemical effects that should therefore be considered in studies of long term sequestration projects.

Porous rocks with fluids: Applications to CO_2 sequestration

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The long-term effectiveness and stability of subsurface sequestered CO_2 accumulations will critically depend on accurate reservoir characterization and subsequent geophysical monitoring of the movement and fate of carbon within the reservoir. The injection of chemically reactive CO_2 bearing brine into a hosting reservoir poses new challenges for modeling and interpreting geophysical observations, particularly when the reactive fluids trigger dissolution or precipitation (*i.e.* porosity enhancement or destruction) both modifying the pore geometry and connectivity of the rock reservoir. Traditionally, physical and chemical processes have been treated as decoupled problems. Thus, current purely mechanical fluid substitution models, treating the properties of the rock frame as invariant with time, are inadequate for quantifying the long-term effects of CO_2-bearing reactive fluids on *in situ* seismic velocities.

The formulation of more comprehensive models, though, requires a fundamental understanding of the combined effects of pore pressure, mineralogy, and of the evolution of pore microstructure on CO_2-fluid-matrix reactivity and, in turn, the effective elastic properties of the formation upon injection. To quantify how the resulting long-term, CO_2-injection-induced changes to *the rock pore space and frame affect seismic parameters in the reservoir*, we developed an approach combining *Experimental and Computational Rock Physics*.

Laboratory measurements of the acoustic, transport, and hydraulic properties of carbonates and carbonate cemented sandstones over a range of confining and pore fluid pressures provides the physical interrelationships between the rock properties and the change of geophysical parameters upon the injection of CO_2 and carbonated brine. Nevertheless, physical interrelationships of rock parameters need to be integrated with a detailed and accurate imaging of the evolution of the rock microstructure occurring upon CO_2 injection. We achieve this via a combination of high resolution (below 1 micron, as needed) and very fast (minutes) imaging of the pore spaces of plugs (e.g. 2D AND 3D CT-scan and SEM images). This combined approach is based on the rigorous understanding of the mechanisms underlying the coupled physical and chemical processes in porous rocks with reactive fluids, and emerging computational codes that efficiently simulate 3D multi-fluid flow (e.g. single- and two-phase flow CO_2) to model CO_2 sequestration at the pore scale while including dissolution/precipitation effects.

Seismic waves in reservoirs with fluids and fractures

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Seismic wave propagation through the earth is often strongly affected by the presence of fractures. When these fractures are filled with fluids (oil, gas, water, CO_2), the type and state of the fluid (liquid or gas) can make a large difference in the response of the seismic waves. Recent work of the PI on deconstructing the effects of fractures, and any fluids within these fractures, on seismic wave propagation as observed in seismic reflection data will be summarized. Methods considered include Thomsen's weak anisotropy approach to seismic wave move-out, crack-influence parameters introduced in the mechanics literature, and poroelastic effects.

Defining and addressing the pressing seismic exploration and production challenges

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When the assumptions behind seismic processing algorithms are violated the result is often misleading or totally erroneous prediction, drilling dry-holes, and the most significant and pressing seismic exploration challenges. It is convenient to catalog three distinct types of seismic processing assumptions: (1) data acquisition, (2) compute requirements and (3) innate algorithmic assumptions. An innate algorithmic assumption violation is defined as occurring under fully adequate acquisition and compute capability. A comprehensive and effective strategy for responding to the pressing and prioritized seismic exploration challenges must begin by recognizing these three distinct types of issues, which separately or collectively need to be addressed.

There are two ways to imagine addressing these assumption violations: (1) develop a new method or capability to satisfy the violated assumption, and (2) develop a new concept and methodology that both in principle or practice avoids and doesn't require the difficult to satisfy assumption.

We feel that adopting one or the other of these two approaches is reasonable under different circumstances. The need for more complete data acquisition and increased compute power demanded by wave theoretic processing methods can be satisfied with advances in more extensive and effective data collection/extrapolation and compute architectures, respectively. In the innate assumption category, there are relatively simple 2D acoustic models where we cannot find an adequate velocity to image a target. There are other simple examples where given a perfect velocity model we cannot wave field extrapolate through that medium to locate even a simple horizontal target reflector. These cases exemplify innate algorithmic breakdown/ limitations of all of our leading edge velocity analysis and imaging tools, under perfect acquisition and compute conditions. The innate algorithmic breakdown can wreak havoc under complex geologic conditions, and is behind many subsalt, sub-basalt and karsted sediment play failures and imaging challenges. The fingering and complex interfaces between injected fluids and oil that occur in 4D, and carbon sequestration applications, present new challenges to imaging techniques due to the rapid variation and geometric complexity of the target.

In this presentation, we will review how the inverse scattering series, and task specific sub-series, represent a direct response to the innate algorithmic break-down described above, and the challenges of removing multiply reflected events and imaging and inverting primaries. The inverse scattering series promises to achieve all processing objectives directly in terms of the measured surface data, and without ever requiring a determination or even an estimation of actual subsurface properties. The current plan is to bring to the extraction of information from primaries, the same high level of effectiveness that the inverse scattering series earlier brought to the removal of coherent noise (multiples). We will illustrate these methods and concepts and capabilities with synthetic and field data. Plans and open issues will be presented.

Fracture characterization using prestack analysis of wide-azimuth seismic reflection data

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Natural fracture networks are largely responsible for the hydraulic conductivity of tight, low-porosity reservoirs. Therefore, reliable estimation of fracture density and orientation is extremely important for cost-effective hydrocarbon production and CO_2 sequestration. An increasingly prominent role in fracture characterization is played by seismic inversion methods that operate with 3D wide-azimuth reflection data. Fracture networks and nonhydrostatic stress fields make the subsurface azimuthally anisotropic and strongly influence such signatures as amplitude-variation-with-offset (AVO) response, reflection-moveout attributes, and the attenuation coefficient.

We developed an advanced methodology for high-resolution AVO analysis of wide-azimuth data from layered azimuthally anisotropic media. A key new element of our processing flow is the moveout-based anisotropic geometrical-spreading correction ("MASC"), which removes amplitude distortions in the overburden and reconstructs the reflection coefficient at the target horizon without knowledge of the velocity model. Amplitude analysis is preceded by nonhyperbolic moveout inversion and estimation of the effective and interval normal-moveout (NMO) ellipses. The moveout parameters not only allow us to flatten long-spread reflection events for the full range of azimuths, but also serve as the input to MASC.

The method was applied to wide-azimuth P-wave data acquired over a fractured gas sand formation at Rulison field, Colorado. Gas production comes primarily from low-porosity channel sand lenses embedded in fine-grained levee deposition. The azimuthally varying AVO gradient, which controls near-offset amplitudes, proved to be the most sensitive fracture-detection attribute. Pronounced azimuthal AVO anomalies were observed for all three processed horizons, which indicate that fracturing is not limited to the reservoir level. In contrast, the moveout attributes both inside the reservoir and in the overburden are weakly dependent on azimuth.

Application of MASC helped to identify two areas of extremely large AVO ellipticity at the bottom of the reservoir. Both anomalies coincide with intersections of wrenching fault systems, where one can expect concentration of stress. Although the fracture orientation estimated from the AVO ellipses varies over the field, the dominant fracture azimuth (N70W) is in good agreement with electrical microimager logs and the direction of one of the fault systems. This geologic evidence strongly suggests that the anomalies correspond to "soft spots" of high fracture density. For purposes of quantitative AVO inversion, P-wave data should be combined with prestack amplitudes of PS- or SS-waves.

Pore-scale simulations of erosion in narrow fractures-new methods and applications

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A fundamental understanding of the role of fractures is an essential component of theoretical models of geological systems. In particular, CO_2 sequestration will require predictive models for the effects of fracture on the overall permeability of rock-fluid systems, and more importantly, how this fracture permeability evolves with time. In fractured rocks, naturally occurring variations in aperture can, under the right flow conditions, cause highly localized erosion. There is a feedback mechanism, which tends to amplify initially small variations in permeability leading to the formation of channels through which almost all the fluid flows. We have previously confirmed that such mechanisms exist independent of order of the erosion kinetics. The goal of our present work is to better understand how aperture variation can promote dissolution breakthrough via flow focusing and if this depends to a significant extent on the density of contact points. We have incorporated a finite-difference solution for the concentration field, which will enable us to study the effects of non-linear kinetics.

Achieving pore-scale resolution of the flow and concentration fields requires large grids. We have replaced the previous height maps with a full 3D geometry, using a novel method of keeping track of the eroding boundaries. Test calculations show that an initially spherical object erodes smoothly and we expect a substantial improvement in the accuracy of the fracture simulations. The flow and transport codes are now fully parallelized, which will allow us to study larger systems and at greater resolution than was possible with our previous serial code. We are currently validating the code by comparison with earlier results, obtained with an implicit Stokes solver and random-walk transport code.

Development of isotope techniques for reservoir and aquifer characterization

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Important issues related to CO_2 sequestration in water-saturated zones are the amount of interstitial pore water, the extent of gas-water interaction and the chemical impact on the reservoir due to CO_2 injection. Modeling predicts that precisely measured details of a chromatographic separation profile for a suite of phase partitioning gases with different solubility would provide important information regarding the extent of gas-water interaction and an integrated gas/H_2O volume ratio. During and after CO_2 injection, temporal and spatial changes in the isotopic compositions of various solutes (e.g. Ca, Sr, Pb, C, O) are expected to trace the occurrence and rates of mineral dissolution and precipitation driven by changes in the chemical attributes of the water-rock system as a result of CO_2 injection. We have field tested the utility of phase-partitioning tracers as part of a CO_2 sequestration experiment in the Frio Formation in the Gulf Coast South Liberty Field, Texas in which noble gases and SF_6 were injected along with the CO_2 stream and monitored downstream. Despite the close proximity of the monitoring and injection wells, which would act to minimize the anticipated chromatographic effect, significant differences in peak arrival times for Kr and SF_6 were observed and an integrated aqueous phase saturation of ~32-45% was calculated. Currently we are formulating field projects in support of the SECARB and WESTCARB demonstration projects, evaluating CO_2-H_2O oxygen exchange as an isotopic measure of gas/water ratios and measuring noble gas solubility in CO_2.

Placing time constraints on recharge and flow of groundwater is an extremely important and difficult problem that affects a wide variety of geologic processes that are relevant to environmental issues, such as water resource management, CO_2 sequestration, waste management, and paleoclimate studies and subsurface water-rock reaction and transport rates. To address these and similar issues, reliable techniques for determining aquifer recharge rates and water residence ages are required. In collaboration with Neil Sturchio, University of Illinois, Chicago and Dr. Zheng-Tian Lu, Physics Division, Argonne National Laboratory, radio-chlorine (^{36}Cl) and radiogenic noble gases (^{4}He and ^{40}Ar) were measured to assess the residence time of old groundwater in the Nubian Aquifer of the Western Desert of Egypt. A systematic increase in the amount of radiogenic ^{4}He that accumulated in the groundwater along the inferred flow path confirmed the age progression indicated by the $^{36}Cl/Cl$ ratios, but a flux of external radiogenic ^{4}He equivalent to ~3.5 times the *in situ* production rate of the aquifer is required to reconcile the ^{4}He accumulation ages with those determined from ^{36}Cl. We are expanding this line of research to include other radio-chronometers, such as ^{81}Kr, by investigating old groundwater from aquifers of the mid-continental United States.

Reactivity of calcite in saline waters

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Sequestration of carbon dioxide into the subsurface is likely to at many potential sites involve interactions with highly saline waters (brines) in carbonate-hosted rocks and carbonate-cemented sandstones. Initial reactions are likely to involve calcite dissolution and subsequent reactions may involve calcite precipitation due to changes in temperature and pressure or mixing with other subsurface waters. It is consequently important to understand the reactivity of calcite in saline waters. Although extensive research has been done on this topic in seawater due to its importance to the marine carbonate cycle, relatively little is know about calcite dissolution, precipitation and nucleation in highly saline waters. Previous work under DOE sponsorship in our laboratory (Gledhill and Morse, 2006) indicated an unexpectedly large influence of ionic strength on dissolution rates, beyond that attributable to its influence on activity coefficients, which led us to the research reported here.

The specific effect of ionic strength on the reaction kinetics of calcite dissolution in intermediate to high ionic strength ($0.5 \leq I \leq 6.0$) solutions applicable to natural waters has been investigated using classical free-drift methods where all other parameters (m_{Ca2+}, P_{CO2}, and T) have been held constant. Both phosphate-free solutions of potassium chloride (KCl) and sodium chloride (NaCl) as the dominant ionic strength determining salt were investigated where calcium concentrations were held constant in all solutions at approximately 0.010 molal. Reaction rates were found to vary significantly as a function of ionic strength of the reacting solution, which we suggest is due to the lowered activity of water with an increase in ionic strength which decreases the rate of cation hydration. When modeled with the general rate equation, $R = k(1 - \Omega)^n$, first-order kinetics (n=1) are sufficient to fit the experimental data. Furthermore, the rate constant (k) appears to be a function of the ionic strength of the reacting solution. The effect of P_{CO2} and T has also been investigated in these same intermediate to high ionic strength solutions where calcium concentrations were held constant in all solutions at approximately 0.010 molal. Dissolution rates increase with either an increase in P_{CO2} or an increase in T. An Arrhenius plot yields an apparent activation energy for this reaction of approximately 20 kJ mol^{-1}.

Nucleation experiments and overgrowth experiments, on Iceland spar calcite, have also been carried out from the same solutions under supersaturated conditions. A surprising finding was that the metastable monoclinic-$CaCO_3$ mineral vaterite initially nucleates in high ionic strength NaCl solutions and rapidly recrystallizes to calcite with excellent rhombohedral grains. Growth on crystals is complex and dominated by a polynuclear "birth and spread" mechanism. Individual crystals are often submicron in size and their arrangement mimics the host crystal's surface morphologic features over multiple growth layers. Recrystallization into larger surface crystals occurs over time periods of weeks to months.

Gledhill, D.K. and J.W. Morse, 2006, Calcite dissolution kinetics in Na-Ca-Mg-Cl brines, Geochimica et Cosmochimica Acta **70**, 5802-5813.

New experimental approaches to mineral surface chemistry and reactivity characterization

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Identifying the major factors and quantifying their influence in the thermodynamics and kinetics of reactions at mineral-water interfaces will significantly improve geochemical models used in reactive transport modeling. The project emphasis includes the elucidation of lateral force contrast mechanisms in the atomic force microscope (AFM) and the study of morphological relaxation in response to solution perturbations. Addressing the mechanisms for lateral force contrast observed on dolomite surfaces in previous studies[1, 2], AFM adhesion measurements and force modulation microscopy (FMM) were used to study monolayer film mechanics on dolomite in aqueous solutions. The major findings in our study of $Ca_xMg_{1-x}CO_3$ films were that the mechanical properties of the film were far more significant in affecting the film friction than was the chemical interactions between the AFM probe and surface. Our working hypothesis was that the relative size of the cations in mixed-cation strained films governs friction forces on carbonate minerals. By investigating Cd- and Sr-rich carbonate films on calcite, we found that both the smaller Cd ion (relative to Ca ion) and the larger Sr ion, when introduced into a carbonate film, both yielded relative increases in friction.

The response of any mineral-water interface to changes in environmental conditions, dissolution and mineralization rates undergo rapid changes as the reaction rates at step edges are governed directly by these environmental changes. These rapid responses at step edges tend to produce "steady-state" reaction conditions with a short relaxation time. However, the production of steps by two-dimensional nucleation is an important factor in the development of "steady-state" surface morphology. Our investigation of celestite, used as a model mineral for these initial studies, have revealed that the topographic relaxation time under near equilibrium conditions approaches days; much longer than the characteristic times of experimental investigations[3].

The LBL (formerly LLNL) part of the project has focused on developing capabilities for the Hydrothermal AFM (HAFM) that are required for the collaboration with WSU. The developments have added the ability to study the connection between stress (mechanics) and chemistry at the mineral/solution interface. We developed a min-bending jig for the HAFM, permitting us to achieve stress intensity factors ranging from 2.5×10^{-2} to 7.2×10^{-1} MPa*m$^{1/2}$. This covers the stress range pertinent to most materials of geologic significance. We redesigned the HAFM to use a longer piezo tube that extends the x-y scan range from 30 to 120 μ and the z-range from 1.2 to 2.3 μ and devised a new Kalrez® membrane shape/composition that has a higher T limit and yet has a lower gas permeability. The new shape uses a pre-formed dimple that lowers stiffness and drag on the piezo. After testing the new HAFM, we made subcritical crack growth measurements and realtime movies of the process in the HAFM under controlled T, P, and fluid chemistry conditions, including switching fluid composition during experiments. Other major design improvements include optical head cooling to prolong the lifetime of expensive commercial optical/electronic components and the implementation of a x-y translation stage for moving the sample over a ± 1mm range, providing the HAFM with nearly the same range in sample positioning as the mechanical stage used by the Digital Instruments MultiMode AFM.

1. Higgins, S.R.; Hu, X., Self-limiting growth on dolomite: Experimental observations with *in-situ* atomic force microscopy, *Geochimica et Cosmochimica Acta* **2005**, *69*, 2085-2094.
2. Higgins, S.R.; Hu, X.; Fenter, P., A quantitative lateral force microscopy study of the dolomite (104)-water interface, *Langmuir* **2007**, *23*, 8909-8915.
3. Bose, S.; Hu, X.; Higgins, S.R., Dissolution kinetics and topographic relaxation on celestite (001) surfaces: The effect of solution saturation state studied using Atomic Force Microscopy, *Geochimica et Cosmochimica Acta* **2008**, *72*, 759-770.

Pyrite surface reactivity under environmentally relevant conditions

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The terrestrial ubiquity of pyrite and its presence in sedimentary basins makes its oxidation a concern during CO_2 sequestration processes. Controlling the acidity resulting from the oxidation of pyrite is a well-appreciated challenge considering the environmental damage due to acid mine drainage resulting from coal mining operations. Indeed some CO_2 sequestration potential protocols call for the injection of CO_2 in to coal seams, which undoubtedly contain pyrite. The general theme of our research is to understand how pyrite reacts in different environments, including those that may cause the oxidative decomposition of the mineral.

Studies will be presented that utilize infrared spectroscopy, probe microscopy, and batch geochemical methods to study the reaction of pyrite in acidic media. Mechanistic information on these goals is a significant focus, along with an appreciation for how this understanding can be used to control the surface reactivity of pyrite in abiotic and biotic environments that promote the decomposition of pyrite.

Results will be presented that show how the surface of pyrite can be functionalized by the adsorption of organic compounds to suppress its propensity to decompose at low pH in abiotic and biotic environments. We feel that the results have potential application in controlling the reactivity of metal sulfides in subsurface and surface environments.

Rates and mechanisms of mineral-fluid interactions at the nanoscale

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The purpose of this effort is to advance our fundamental understanding of rates and molecular-level mechanisms of mineral-fluid reactions both near and far from equilibrium, over the full range of temperatures and compositions encountered in near-surface shallow crustal environments. Determination of the rates of dissolution-precipitation and isotopic exchange at variable departures from equilibrium are coupled with a mechanistic description of the initiation of reactions at reactive surface sites. Detailed investigation of the formation of, and chemical communication across, leached layers and reaction zones, and the structure and dynamics of fluid species present in porous reacted solids will contribute to a more complete understanding of equilibrium/disequilibrium processes preserved in mineralogical record resulting from water-rock interaction. We have measured the rates of dissolution and precipitation near- and very-near equilibrium that utilizes our unique, high temperature, *in situ* pH measurement facilities. We have also interrogated the nature of porosity generation and its role in fluid transport and confinement dynamics in mineral reaction zones using advanced chemical and isotopic imaging approaches (e.g. secondary ion mass spectrometry, neutron scattering, and others) coupled with modeling and simulation.

The dissolution/precipitation rates of boehmite, AlOOH, at 100.3°C and limited dissolution kinetics of gibbsite, $Al(OH)_3$, at 50.0°C were measured in neutral to basic solutions at 0.1 molal ($mol \cdot kg(H_2O)^{-1}$) ionic strength (NaCl) near equilibrium using a pH-jump technique with a hydrogen-electrode concentration cell. This approach allowed relatively rapid reactions to be studied from under- and over-saturation by continuous *in situ* pH monitoring after addition of basic or acidic titrant, respectively, to a pre-equilibrated, well-stirred suspension of the solid powder (an initial period of time was required for temperature stabilization and electrode response before the kinetics could be followed). The magnitude of each perturbation was small to maintain close to equilibrium conditions. In collaboration with researchers at Penn State (Sue Brantley, Karl Mueller, Mike Davis) we have also investigated the equilibrium solubility and the very-near-equilibrium dissolution rates of quartz, SiO_2, and forsterite, Mg_2SiO_4, in acidic and basic NaCl brines from ambient conditions to 150°C using this approach. We have demonstrated that both the equilibrium solubility and the dissolution rates of quartz in basic solutions can be determined without the need for sampling the solutions. The kinetics of forsterite dissolution suggest that initial leaching of Mg^{2+} by proton exchange is followed by expulsion of H^+ due to polymerization of silica in the leached layer. This process was accompanied by formation of a minor secondary phase at the higher temperatures which we have recently interrogated with neutron diffraction experiments at NIST.

In concert with high resolution TEM studies we have explored the application of SANS and USANS to interrogate the development of secondary porosity in natural materials, in this case weathered basalt clasts (with collaborators from PSU), limestones that have experienced thermal alteration (with UTK), and hydrothermally altered feldspars. Results from the weathered basalts indicate the presence of micropores and mesopores with the former exhibiting surface fractal features whereas the latter exhibit mass fractal features. Similar fractal behavior was observed in the altered limestones and feldspars.

We used backscattering neutron spectroscopy (QENS) to probe the dynamics of water mobility in LiCl and $CaCl_2$ aqueous solutions confined in 2.7, 1.9, and 0.9 nm pores of various silica matrices. The pore size of 2.7 nm was found to be sufficiently large for the confined liquids to exhibit characteristic traits of bulk behavior, such as a freezing-melting transition and a phase separation. On the other hand, none of the fluids in the 0.9 nm pores exhibited a clear freezing-melting transition; instead, their dynamics at low temperatures gradually become too slow for the nanosecond resolution of the experiment. The mobility of water was suppressed the most in the $CaCl_2$ solutions, indicating the influence of the cation charge on the dynamics of the water molecules. QENS measurements of pure H_2O and 1 M LiCl-H_2O solution confined in 1.9 nm pores revealed a dynamic transition in both liquids at practically the same temperature of 225-226 K, even though the dynamics of the solution at room temperature appeared to slow down by more than an order of magnitude compared to the pure water. The observation of the dynamic transition in the solution suggests that this transition may be a universal feature of water governed by processes acting on the local scale, such as a change in the hydrogen bonding.

Poster Session Abstracts from RCSP and SciDAC

Big Sky Regional Carbon Sequestration Partnership (Big Sky)
Plains CO_2 Reduction Partnership (PCOR)
Midwest Geological Sequestration Consortium (MGSC)
Midwest Regional Carbon Sequestration Partnership (MRCSP)
Southeast Regional Carbon Sequestration Partnership (SECARB)
Southwest Regional Partnership on Carbon Sequestration (SWP)
West Coast Regional Carbon Sequestration Partnership (WESTCARB)
NATCARB
NETL Geologic and Environmental Focus Area
SciDAC posters

Big Sky Regional Carbon Sequestration Partnership Phase II overview and Phase III large scale demonstration project

The Big Sky Carbon Sequestration Partnership (BSCSP) is one of seven of NETL's regional carbon sequestration partnerships. The primary goal of the BSCSP is to promote the development of a regional framework and infrastructure required to validate and deploy carbon sequestration technologies. BSCSP's work focuses on improving the understanding of factors affecting CO_2 storage, permanence, capacity, and safety in geological and terrestrial ecosystems. The BSCSP research also analyzes the policy and regulatory frameworks, economics and infrastructure needs to deploy the developing technologies at a commercial scale. The BSCSP has Phase II geologic efforts involving a small volume injection in mafic rocks and a study of naturally occurring CO_2 reservoirs in southwestern Wyoming and geologic domes of Montana. Several terrestrial sequestration projects are in progress to spawn the development of carbon markets and to evaluate lower cost validation efforts. The BSCSP is planning a large volume sequestration test to demonstrate geologic storage of carbon dioxide in southwest Wyoming as part of its Phase III effort.

BSCSP's Phase III project will perform a large volume sequestration test in the Triassic Nugget Sandstone Formation on the Moxa Arch. The test will inject one million tons of CO_2 per year for three to four years into the saline aquifer at depths of 12,000 feet. The Nugget sandstone is equivalent to the Tensleep, Weber, and Navajo formations, that have been identified as regionally extensive sequestration targets in the western US. The carbon dioxide will be supplied by Cimarex Energy from their gas plant in the Riley Ridge Field. The Cimarex plant, scheduled for completion in late 2008 or early 2009, will extract methane and helium from gas produced from the Madison Limestone at 18,000 feet. The produced gas is 75% carbon dioxide with accompanying methane, hydrogen sulfide and helium. The non-economic portion of the gas will be re-injected back into the deep Madison Limestone. The plant will produce approximately 1.5 million tons of high pressure CO_2 per year. The CO_2 for the project (92% CO_2 and 8% H_2S) will be diverted in a short lateral pipeline for injection into the Nugget Formation on Cimarex Energy lease holdings. Information from the project will be used by Cimarex Energy to evaluate the potential to establish a commercial sequestration facility.

The planned injection site occurs west of LaBarge, Wyoming and is east of the thrust belt that creates the LaBarge Platform and Moxa Arch geological features. Total thickness of the Nugget Sandstone in the area of LaBarge is approximately 700 feet. The formation is highly permeable, and has an average porosity of greater than 15%. Land ownership is a mix of public and private lands with the largest proportion of lands under management of the United States Department of Interior's Bureau of Land Management (BLM).

The major research objectives are to: 1) evaluate the Nugget Sandstone saline aquifer responses to injection of large volumes of supercritical CO_2; 2) track the post-injection migration and containment of the CO_2 in the Nugget Sandstone Formation to compare with pre-injection reservoir modeling predictions and to serve as a basis to refine predictive models; and 3) evaluate the performance of MMV procedures used during the project.

Plains CO_2 Reduction Partnership

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Over 70 partners from industry, government, and nongovernment organizations contribute time, resources, and expertise to the Plains CO_2 Reduction (PCOR) Partnership. The region contains vast energy, agricultural, forest, and water resources and offers significant opportunities for both geologic and terrestrial sequestration. Three geologic field validation tests and one terrestrial test are now under way in Phase II, while two large-scale demonstration tests are planned in Phase III.

Apache Canada Limited is hosting a combined enhanced oil recovery (EOR)–sequestration activity that is injecting acid gas (approximately 70% CO_2 and 30% H_2S) from the Zama, Alberta, gas plant for use in a miscible flood and for sequestration. CO_2 injection into Devonian pinnacle reef structures in the Zama oil field in northwestern Alberta, Canada, has been occurring since December 2006 at an average rate of approximately 50 tons of CO_2 per day. The project is focused on examining the effects that high concentrations of H_2S can have on EOR and carbon sequestration operations, particularly with respect to monitoring, mitigation, and verification (MMV).

An EOR project in the North Dakota portion of the Williston Basin has been designed to demonstrate the potential of using CO_2 in a tertiary oil recovery operation at depths of approximately 10,000 feet. The Williston Basin field validation test is developing the geological characterization data as a precursor to the full development of a commercial-scale sequestration demonstration in Phase III. Thus far, significant geological characterization data and models have been developed to help our commercial partners with site selection and preliminary engineering analysis of candidate sites.

The potential for CO_2 sequestration and enhanced-coalbed methane production in Williston Basin (Burke County, North Dakota) lignite is being investigated to evaluate the features of fluid transport in lignite, the stability of carbon dioxide stored within a lignite seam, the factors controlling the success of sequestration/methane production operations in lignite, and the economics of the operation. Thus far, the lignite field validation test has drilled a five-spot production/injection well geometry to allow for efficient site characterization, CO_2 injection, and MMV activities. A significant suite of geophysical logging techniques was utilized, and core of the targeted coal was collected for analysis in order to develop an injection and MMV strategy to be employed in the spring of 2008.

A terrestrial field validation test (McPherson County, South Dakota) is under way to develop carbon offsets from alternate management of wetlands in the Prairie Pothole Region (PPR). Work thus far has focused on demonstrating optimal practices for sequestering CO_2 through the restoration of PPR wetlands and surrounding grasslands at a site in north-central South Dakota. The project results are intended to serve as a model to promote and implement terrestrial sequestration across the PPR.

Phase III includes a saline aquifer injection in the Alberta Basin (1.8 million tons per year) and a combined sequestration–EOR project in the Williston Basin (0.5–1.0 million tons per year). The CO_2 source for the Alberta Basin project is an acid gas-processing facility, while a retrofitted conventional coal-fired power plant will provide the CO_2 for the Williston Basin demonstration.

Planning and implementation of Phase II EOR and ECBM pilot projects and the Phase III (ADM) saline sequestration validation site

Midwest Geological Sequestration Consortium

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Development and evaluation of a reservoir model that utilizes pre-drill estimates of design criteria, such as injection rate and pressure, are needed for site selection, well construction, surface facility design and a comprehensive MMV program. Phase II research included implementation of pilot injection programs for EOR and ECBM applications. For the Phase III sequestration demonstration project in the Illinois Basin, the target is the Cambrian Mt. Simon Sandstone, a thick (over 2,600 feet in places) sandstone reservoir. The planned site is at Archer Daniels Midland (ADM) Company Decatur, Illinois ethanol fermentation facility.

Because there are no Mt. Simon penetrations within a 17-mile radius of the planned site, regional geology and distant wells were used to best model the local conditions. Reservoir flow modeling suggests that after injection of one million tonnes of CO_2 in a lower Mt. Simon interval, the plume would not have reached the overlying Eau Claire, the primary seal above the Mt. Simon and the plume would extend laterally less than 1,500 feet. The proposed injection well will be drilled in the summer of 2008 to the Precambrian granite basement for an approximate total depth of 7,900 feet.

A comprehensive MMV program has been planned for the ADM sequestration site. They include a full gamut of geophysical methods such as 3D seismic, VSP profiles, and passive seismic monitoring. Geochemical and near-surface methods include soil gas sampling, isotopic composition analysis, CO_2 land surface flux monitoring, and visible and infrared imaging. Shallow ground water monitoring will be used pre-injection, during injection, and post-injection to measure quality and flow direction in shallow ground water.

Accomplishments to date on the Phase II projects include a Huff'n Puff injection of CO_2 in the Owens lease within Louden Oil Field. Results indicate that CO_2 pattern flood of Illinois Basin oilfields may successfully increase oil production. A four-well ECBM pilot project has been started in Wabash County, IL, where coal core desorption analyses, COMET modeling, and pressure transient analyses for the initial two wells shaped the design of the pilot that should be ready for CO_2 injection in spring of 2008. Phase III progress at the ADM site includes 2D seismic acquisition and interpretation, and submittal of the UIC permit application to the Illinois EPA.

The Mt. Simon was selected as the optimum saline sink for the Phase III validation test because of its widespread nature and the immediately overlying Eau Claire shale as a seal. The Mt. Simon underlies one of the largest concentrations of coal fired power plants in the world. This makes the Mt. Simon one of the most significant carbon storage resources in the United States.

Understanding the geologic storage potential in the midwestern USA through multiple field demonstrations

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The eight states comprising the Midwest Regional Carbon Sequestration Partnership (MRCSP) represent a large fraction of the U.S. economy with a dependence on fossil fuel based energy and the resulting CO_2 emissions. These states are also endowed with a large and diverse potential for CO_2 storage in deep saline formations, oil and gas fields, shale layers, and coal seams. This geologic diversity includes the presence of two mature deep basins, the Michigan basin in the north and Appalachian basin in the center of this region; the uplifted arches region in Ohio, New York, Kentucky, and Indiana; and Appalachian Valley and Ridge, crystalline Blue Ridge, Piedmont provinces and the Coastal Plains sediments in the eastern part of MRCSP. Validation of geologic storage potential in this area requires continued regional geologic exploration along with site-specific demonstrations of integrated CO_2 injection and monitoring – both part of MRCSP's ongoing Phase II and planned Phase III efforts. The diverse geologic features of the region are reflected in three small-scale tests being conducted in the Michigan Basin, Appalachian Basin, and Cincinnati Arch regions, as well as the planned larger-scale demonstration under Phase III. Equally importantly, these tests are being conducted in collaboration with energy companies that are the potential future users of geologic sequestration technology. Each field test incorporates extensive characterization, permitting, reservoir modeling, outreach, injection, and monitoring, as discussed below:

Saline Reservoir Injection at Duke Energy's East Bend Plant in Kentucky – This area represents the uplifted arches geologic province that separates the Illinois Basin from the Appalachian Basin. The most likely injection zone in this area is the Mt. Simon Sandstone (~100 m thick and ~1,200 m deep) although other high permeability zones are likely to be present above (Knox Dolomite) or below (Middle Run Formation) this interval. There is excellent containment in this area and overall injectivity is likely to be very high. The site is representative of a large part of the MRCSP Region and an explicit linkage to current or potential future power plants makes it attractive for deployment at full-scale in the future. A background geologic assessment, 2-D seismic survey, initial outreach, and permit preparation for the site have been completed. An injection well and potentially an observation well will be drilled after permitting is complete, followed by injection and monitoring of about 3,000 tonnes of CO_2 from a commercial supplier. A site-specific suite of monitoring options is being finalized.

Saline Reservoir Injection using CO_2 from a DTE Gas Processing Plant in the Michigan Basin – Several gas processing plants in the northern part of the Michigan Basin produce a pure CO_2 stream and one of these source plants operated by DTE Energy has an associated compression plant and local pipeline infrastructure for EOR operations being carried out by Core Energy in Silurian carbonate reefs at a depth of about 1,500 meters. Injection of CO_2 for the MRCSP test will be in dolomitic saline formations at about 1,100 meters depth. Site characterization, outreach, baseline monitoring in injection and monitoring wells, permitting, and construction at the site are already complete. Injection of approximately 10,000 tonnes of the CO_2 will take place during February-March 2008. The monitoring techniques being used at this site include cross well seismic, borehole micro-seismic, PFT tracers tests, wireline logging including fluid saturation profiles, fluid sampling, and continuous pressure-temperature monitoring.

Saline Reservoir Injection at FirstEnergy's R.E. Burger Plant in the Appalachian Basin – This relatively unexplored site provides an opportunity to test multiple injection zones, which are typical of many parts of Appalachian Basin, for geology, containment, and injectivity. A 2-D seismic survey of the area has been completed along lines intersecting the location of a ~2,500 meter deep test well that was completed in early 2007 at the Burger plant grounds. An injection well permit is currently being processed by Ohio EPA. Approximately 3,000 tonnes of CO_2 will be injected during mid to late 2008, using commercial CO_2 or, if feasible, CO_2 from an aqueous ammonia based CO_2 capture technology being tested at the plant. The monitoring techniques used for this site will be based on a single well test, because no monitoring wells are likely to be available at this site.

MRCSP Phase III Large-Scale Injection Test – Consistent with DOE's accelerated schedule for conducting large-scale demonstration at multiple locations, MRCSP has proposed using CO_2 from an ethanol plant in western Ohio for on-site injection of at least 250,000 tonnes of CO_2 per year for four years. This test will be conducted in the Cincinnati Arch province, with the Mt. Simon Sandstone as the injection zone at a depth of about 1200 meters with a regional shale, the Eau Claire Shale, as the primary caprock. The site plans include construction of a compression plant, on-site pipeline, one or more injection wells, monitoring wells along with deployment of a comprehensive suite of monitoring options. Injection is scheduled to start by 2010.

Conclusions – The key issues related to implementation of the CCS technologies in the MRCSP region are evaluated through regional mapping followed by selected injection tests that represent the geologic diversity of the region. The MRCSP tests allow for validating the geologic storage potential in key formations and testing the applicability of monitoring technologies in differing geologic settings. They also include a strong linkage to CO_2 sources, regulatory and outreach issues, and field deployment aspects. Finally, the MRCSP efforts involve partnering with key regional stakeholders whose acceptance is crucial to large-scale technology deployment.

Southeast Regional Carbon Sequestration Partnership (SECARB) – Moving from field test implementation to deployment phase

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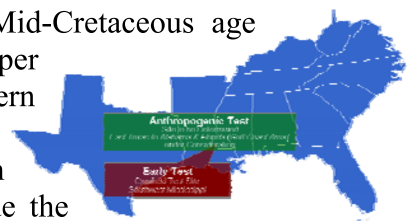
Background: The Southeast Regional Carbon Sequestration Partnership (SECARB), led by the Southern States Energy Board (SSEB), represents 11 southeastern states and is comprised of more than 100 research partners and participants. The Partnership estimates that 31 percent of the Nation's CO_2 stationary source emissions come from these 11 states. SECARB's deep saline formations offer potential capacity for safe and permanent storage of those emissions.

Injection Site Description- Early & Anthropogenic: The Early Test will be conducted in the down dip "water leg" of the Cranfield unit, operated by Denbury Resources, Inc. near Cranfield, Mississippi. The Early Test site is immediately north of the SECARB Validation Phase II "Stacked Storage" study underway in the oil rim. The Anthropogenic Test will be conducted at or near a Southern Company plant site in the Gulf Coast region. In 2008, a Field Test of saline reservoir storage will be conducted on the Mississippi Power Company (Southern Co. subsidiary) Victor J. Daniel Power Plant site in Jackson County, MS. A test volume of pure CO_2 will be injected into a deep (>8500 feet) saline reservoir of the Lower Tuscaloosa Formation underlying the power plant site. The Plant Daniel Field Test provides the opportunity to collect reservoir data otherwise unavailable yet essential to the success of the future Anthropogenic Test.

Description of Geology: The Tuscaloosa Formation is one of the numerous sandstone and shale formations that form the Gulf Coast sedimentary wedge. Mid-Cretaceous age sandstones occur at suitable depths beneath much of the upper Gulf Coast along the Gulf of Mexico coastal plain from western Florida to Texas. In the study areas, fluvial-deltaic-paralic sandstones of the lower Tuscaloosa typically have high permeability (up to a Darcy) and porosity (25%) and provide the main injection zone. Injection strategy will take advantage of multiple sandstones with interbedded shales. For the Anthropogenic Test the target storage reservoir is the "Massive" sandstone, a thick, regionally extensive and porous and permeable coastal to deltaic-marine sandstone at the base of the lower Tuscaloosa. Regionally the lower Tuscaloosa is overlain by a thick section (300-450 ft) of shales and mudrocks that were deposed as sea level rose during marine transgression. This low permeability interval provides the major seal above the injection zone, although numerous overlying sandstone-shale and chalk intervals provide redundancy in isolation of the CO_2.



Source of CO_2 and Injection Operations: Injections will be at a scale sufficient to validate model predictions at high and sustained rates, adding confidence to the estimates of injectivity and capacity for future large scale commercial sequestration. The CO_2 source for the Early Test was selected to provide high injection rates, at low cost and in the near term. Denbury Resources will provide 1 million tons/year of CO_2 from a natural source at Jackson Dome (MS) via commercial pipeline. Distribution lines and compression will be developed by Denbury to bring CO_2 from the separation plant to the injection wells. The source of injected CO_2 for the Anthropogenic Test will be a pilot unit capturing CO_2 from flue gas produced at the power plant. The CO_2 will be compressed to 2000 psig and transported a short distance to the injection site.

Reservoir Simulation and Monitoring of Injection: SECARB will conduct rigorous monitoring and model verification during the 10-year project with an array of multiple tools deployed at each site. The project team will simulate flow in rock-water-CO_2 reaction using GEM-CO_2 and TOUGHREACT. Monitoring data will be collected to verify the correctness of the models in predicting plume evolution and determining the ultimate fate of the injected CO_2. The Early Test will focus on measurement of reservoir pressure response and sweep efficiency by saturation measurements at wells and through interwell techniques using 4 injection wells and 2 observation wells. Monitoring activities for the Anthropogenic Test are designed to accomplish the following: (1) assure well bore integrity by using Ultrasonic Imaging Tool (UIT) logging, annular pressure monitoring, and tracer injection; (2) assure safe rates of CO_2 injection by monitoring downhole reservoir pressure and temperature; (3) monitor CO_2 plume movement with up-gradient observation wells, seismic surveys, and the Reservoir Saturation Tool (RST); and (4) early detection of CO_2 seepage using RST logging, and the VSP, and through shallow subsurface monitoring for CO_2, carbon isotopes, and tracers.

Southwest Regional Partnership on Carbon Sequestration: Phase III deployment

Sedimentary basins throughout the Southwest Partnership (SWP) region possess several deep saline formations that are common to most or all basins. Among these are several Jurassic (206 to 144 million years old) and Triassic (248 to 206 million years old) sedimentary units, ranging from the Jurassic Entrada Formation down deeper to the Triassic Wingate formation. These permeable rock formations are present in every state in the Southwest Region; indeed, they are ubiquitous throughout the PCOR and Big Sky Partnership regions as well.

The SWP is designing a deep saline sequestration deployment with injection of ~1 million tons per year for multiple years in these formations within the southern Uinta basin of central Utah. We will conduct a second sequestration deployment of 25,000 – 100,000 tons, also in one or more of these Jurassic-Triassic units, within the Green River basin of southwestern Wyoming. These two geological sequestration tests will provide baseline data necessary to quantify and qualify storage capacity and monitoring requirements associated with future commercial-scale sequestration. Several new power plants are planned for the region, and the Utah and Wyoming test sites possess geological storage reservoirs identical to those underneath all proposed possible IGCC plant sites. A major objective of these analog-site deployments is to develop meaningful "blueprint" plans for commercial-sequestration in the region.

WESTCARB field pilot CO_2 injection tests

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The West Coast Regional Carbon Sequestration Partnership (WESTCARB) is evaluating the geologic sequestration opportunities in the west coast of North America. The project involves three phases.

In Phase I of the project, regional-scale assessments were carried out to identify sedimentary basins with potential for storage, collect data on structure and reservoir properties, calculate storage capacities, as well as to evaluate the regulatory environment, public perception and risks. In Phase II of the project, small volume CO_2 injection tests will be conducted at two locations representative of major sequestration opportunities in the region. The first pilot is planned for a site in the Sacramento Basin in Northern California, and involves injection of up to 4000 tons of CO_2 into a stacked gas and saline formation reservoir. The second pilot will be carried out at a site on the Colorado Plateau in Arizona and will involve injection of about 2000 tons. The goals of the pilots are: demonstrate the feasibility and safety of CO_2 storage in formations representative of major geologic sinks; obtain site specific information to improve capacity estimation, risk assessment, and performance prediction; demonstrate and test methods for monitoring CO_2 storage; and gain experience with regulatory permitting and public outreach associated with CO_2 storage. The California pilot has the additional goal of testing the feasibility of Carbon Sequestration Enhanced Gas Recovery (CSEGR) associated with the early stages of a CO_2 storage project in a depleted gas field.

The primary technical objectives of the Phase II pilots are to assess seal integrity, spatial extent of the CO_2 in the subsurface, and injectivity and storage capacity of the formation. An additional objective of the gas reservoir test is to assess mixing and CH_4 displacement. The California pilot will utilize an injection and observation well. Reservoir simulation and geomechanical analyses predict plume development and stress changes resulting from injection. Vertical Seismic Profiling (VSP) and possibly cross-well seismic will be used to image the plume. A comprehensive suite of wireline logs will augment these geophysical measurements. Injection rates, wellhead and formation pressures will be monitored continuously. Fluid and gas composition will be monitored using samples collected during the CO_2 injection to track migration and allow evaluation of flow and transport processes. The Arizona pilot, which will be carried out at a greenfield site, will involve a single well. This well will first be used as an exploration well to verify the suitability of the subsurface properties, and then as an injection well.

The WESTCARB Phase III project will be a commercial scale test of carbon capture and storage (CCS) in California. It will involve injection of 1M tons of CO_2 over four years into the San Joaquin basin. The project will seek to demonstrate the viability of the basin as a major storage target in the region, and to demonstrate commercial scale sequestration methodologies for site characterization and monitoring. Research will be carried out to support the commercial scale activities and advance technologies in reservoir engineering, risk assessment and monitoring. The project will exercise and provide experience for, evolving regulatory and legal frameworks. Primary technical objectives and approaches are similar to those of the Phase II pilots, with differences in scale taken into consideration.

NatCarb: The beginning of a national carbon cyberinfrastructure

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The NATional CARBon Sequestration Database and Geographic Information System **NatCarb** provides national coverage across the Regional Carbon Sequestration Partnerships (RCSP's). The RCSP's and **NatCarb** have created and maintain the only carbon sequestration portal for matching CO_2 sources with nearby sinks—geologic and terrestrial sequestration sites—in the United States and Canada. **NatCarb** provides an Internet portal that brings together data from every partnership, national data layers, and selected publicly accessible servers (e.g., USGS, and Geography Network) into a network of regional carbon sequestration atlases for North America. The data available from the RCSP's is organized and enhanced through NatCarb and has contributed to creation of the US Department of Energy National Energy Technology Laboratory's *Carbon Sequestration Atlas of the United States and Canada*. The RCSP's and others use the data to identify promising sequestration opportunities; and raise awareness and support for carbon sequestration as a greenhouse gas mitigation option, both within industry and the general public. At the national level water geochemistry data from national and regional data bases have been assembled and linked to an improved set of capabilities for query, visualization and analysis. These visualization and analysis tools are available for aquifers at a national, regional or local scale. The NatCarb portal is updated regularly by region, and is moving to improve public access using commonly available tools such as Google Earth®. NatCarb data and maps are available to decision makers and the general public through a single website (http://www.natcarb.org/).

Geologic Research Performed at the National Energy Technology Laboratory

David Wildman

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NETL's Geologic and Environmental Focus Area conducts research and analysis to develop energy-efficient and cost-effective methods to sequester CO_2 emissions from fossil fuel energy production. This work is: (1) expanding the options to help meet near-term goals for reducing greenhouse gas intensity; (2) ensuring the readiness of future technologies (to meet the 2012 reassessment required by the Global Climate Change Initiative); and (3) making the longer-term goal of greenhouse gas emission stabilization more achievable. NETL's Office of Research and Development has established the Focus Area to conduct research in the areas of permanent storage and assessment of risk associated with permanent storage.

A major initiative of the Focus Area is identifying adequate storage sites (or "sinks") for the CO_2 — places where CO_2 can be stored for several hundred or even thousands of years. The storage must have low environmental impact and low cost, and conform to national and international laws. Primary underground storage options include depleted oil and gas reservoirs, deep saline formations, and unminable coal seams. Researchers in the focus area have been working closely with the Carbon Sequestration Regional Partnerships, providing technical assistance and guidance in selecting sites and answering key site-specific questions related to storage capacity. A suite of modeling techniques is being developed to quantify CO_2 flows near the surface, through intermediate strata, and in deep subsurface sinks. The Focus Area is developing techniques and computer models that will be used by the Regional Partnership participants to verify long-term storage acceptability of geologic formations that are representative of potential storage options in many other locations. Based on recent assessments, the United States has an estimated 230 candidate geologic storage sites. The Focus Area is developing several types of verification techniques, including soil CO_2 flux measurements, groundwater sampling and analysis, aeromagnetic flyover surveys for existing and abandoned wells, characterization of surface fault exposures, core flow analysis using specialized equipment at NETL, CT-scanning of cores to assess fractures and rate of diffusion of CO_2 into the strata, and adsorption isotherm studies of relevant strata. The models being developed and refined include near-surface modeling of CO_2 flow to aid in design and interpretation of monitoring networks, in conjunction with statistical techniques; modeling of flow through actual fractures to better understand flow phenomena; development of unique fracture generation and flow simulation software to model flow through intermediate strata; and simulation of migration through the target formation.

The Focus Area is developing a plan to identify risks associated with the permanent sequestration of CO_2. Using the features, events, processes, and models that have been developed for risk assessments elsewhere as a basis, one key component of the risk assessment activity will be to identify the risks associated with a "sample" field project being undertaken by one of the Regional Partnerships. This approach will tie modeling and monitoring techniques to the risk assessment model, in order to identify potential events, and probabilities of events, that affect CO_2 storage. Development of a carbon storage risk assessment capability will provide a very useful tool that will be used to support the performance of environmental assessments and impact studies of carbon capture and long-term storage options. Results of risk assessments also could be used to inform the public about the safety of carbon sequestration.

Hybrid numerical methods for multiscale simulation of subsurface biogeochemical processes

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Many subsurface flow and transport problems of importance today involve coupled non-linear flow, transport, and reaction in media exhibiting complex heterogeneity. Deep subsurface sequestration of carbon dioxide can lead to the precipitation and/or dissolution of mineral phases that will be strongly coupled to flow and transport processes through modification of the porous media structure. Recent experimental research has revealed important details about some of the physical and chemical mechanisms involved in these processes at local scales (e.g., the pore scale). However, translation of detailed knowledge at small scales into reliable predictions of field-scale phenomena remains challenging. A large assortment of numerical simulation tools have been developed, each with its own characteristic scale. Important examples include 1. pore-scale simulations (e.g., lattice-Boltzmann, pore network models, and discrete particle methods such as smoothed particle hydrodynamics); and 2. macroscopic continuum-scale simulations (e.g., traditional partial differential equations solved by finite difference or finite element methods). While many problems can be effectively addressed by one of these models at a single scale, some problems may require explicit integration of models across multiple scales. We are developing a hybrid multi-scale subsurface reactive transport modeling framework that integrates models with diverse representations of physics and chemistry at different scales (sub-pore, pore and continuum). The modeling framework is being designed to take advantage of advanced computational technologies including parallel code components using the Common Component Architecture, parallel solvers, gridding, data and workflow management, and visualization. This poster describes the specific methods/codes being used at each scale, techniques used to directly and adaptively couple across model scales, and preliminary results of application to a multi-scale model of mineral precipitation at a solute mixing interface.

The next-generation massively parallel reactive flow and transport code PFLOTRAN: Application to CO_2 storage in saline aquifers

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The next-generation multiphase-multicomponent reactive flow and transport code PFLOTRAN is currently being developed under a SciDAC-2 project entitled: *Modeling Multiscale-Multiphase-Multicomponent Subsurface Reactive Flows using Advanced Computing*. PFLOTRAN is a parallel multiphase flow and multicomponent reactive transport model written from the ground up employing PETSc data structures and solvers for its parallel framework. The code employs domain decomposition for parallelization and implements an efficient parallel I/O through HDF5. The code is written in FORTRAN 90 and highly modularized using linked lists, type structures and pointers. Recently, PFLOTRAN has been run on a one billion node real-world problem (Hanford 300 Area) as proof-of-concept for petascale computing. The code ran successfully on 1024 cores on ORNL's Jaguar Cray XT3 computer. The code has also demonstrated a relative parallel efficiency of 79% at 12,000 cores based on a strong-scaling study performed with a similar 500 million node problem executed on 3,000-12,000 cores.

The code is currently being applied to investigate sequestration of CO_2 in various geologic media including depleted oil reservoirs and saline aquifers as a possible solution to reduce green house gas emissions. Dissolution of supercritical CO_2 in formation brines is considered an important storage mechanism to prevent possible leakage. Accurate prediction of the plume dissolution rate and migration is essential. Analytical analysis and numerical experiments have demonstrated that convective instability (Rayleigh instability) has a crucial effect on the dissolution behavior and subsequent mineralization reactions. Global stability analysis indicates that a certain grid resolution is needed to capture the features of density-driven fingering phenomena. For 3-D field scale simulations, high resolution leads to large numbers of grid nodes, unfeasible for a single workstation. In this study, we investigate the effects of convective instability on geologic sequestration of CO_2 by taking advantage of parallel computing using PFLOTRAN. The onset, development and long-term fate of a supercritical CO_2 plume will be resolved with high-resolution numerical simulations to investigate the rate of plume dissolution caused by fingering phenomena.

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