

Zero Emissions Research and Technology
(ZERT) II – Investigating the Fundamental
Scientific Issues Affecting the Long-term
Geologic Storage of Carbon Dioxide
Project Number DE-FE0000397

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Energy Research Institute
Montana State University

U.S. Department of Energy
National Energy Technology Laboratory
Carbon Storage R&D Project Review Meeting
Developing the Technologies and Building the
Infrastructure for CO₂ Storage
August 21-23, 2012

Benefit to the Program

Program goals being addressed.

- Develop technologies that will support industries' ability to predict CO₂ storage capacity in geologic formations to within ± 30 percent.
- Develop technologies to demonstrate that 99 percent of injected CO₂ remains in the injection zones.
- Conduct field tests through 2030 to support the development of BPMs for site selection, characterization, site operations, and closure practices.

Project benefits statement.

ZERT II supports Storage Program goals by **1) developing computational tools for simulating CO₂ injection, storage and trapping, 2) performing basic geoscience experiments to address relationships between properties such as wetting, relative permeability, saturation, and capillary pressure that will improve understanding of CO₂ behavior in the reservoir and help with model parameterization 3) investigating analogs to understand risks to storage security 4) conducting field experiments to test near surface monitoring technologies and 5) developing novel bio-controlled leakage mitigation technology**

Project Overview:

Goals and Objectives

Biofilms and Biomineralization

- Objective: Perform a comprehensive evaluation of techniques for current and novel CO₂ sequestration concepts associated with microbial biofilms.

Natural Analogs of Escape Mechanisms

- Objective: Characterize the physical, mineralogical, and geochemical characteristics of a fracture system that may have been exposed to naturally occurring sub-surface CO₂, for the purpose of determining the reservoir and trap conditions that contribute to long-term CO₂ sequestration versus those that contribute to CO₂ leakage.
- Objective: Characterize the physical, mineralogical, and geochemical characteristics of outcrops of hydrothermal plume related rocks to determine their usefulness as natural analogs of breached and healed caprocks for carbon sequestration.

Optical Detection for Carbon Sequestration Site Monitoring

- Objective: Demonstrate the feasibility of creating an in-line fiber optic sensor for CO₂ that utilizes sections of photonic bandgap (PBG) fibers interspersed with sections of single mode optical fiber.
- Objective: Develop a custom-designed multispectral imager to detect CO₂-induced plant stress with lower cost to allow field deployment of multiple imagers for monitoring large, distributed carbon sequestration facilities.

Validation of Near-surface CO₂ Detection Techniques and Transport Models

- Objective: Determine, via field experimentation, the efficacy and detection limits for existing and emerging near-surface CO₂ detection technologies.

Project Overview:

Goals and Objectives

Task 2.0 – Biofilms and Biomineralization

- Decision Point – Results of pulsed flow experiments concerning ability to control deposition rate and spatial distribution of biofilm barriers.
- Success Criteria – Ability to provide a spatial distribution over an area greater than one inch from in-flow side of porous media.

Task 3.0 – Natural Analogs of Escape Mechanisms

- Decision Point – The geologic outcrop studies must produce enough data to make time investment of development of a three-dimensional static model.
- Success Criteria – One hydrothermal plume of sufficient detail has already been identified, so success is highly probable. The key issue here is determining which plume provides the most appropriate information. We will discuss this with other geoscientists and modelers to make this determination.

Task 4.0 – Optical Detection for Carbon Sequestration Site Monitoring

- Decision Point – Demonstration of the ability to re-launch light into subsequent fiber sections when an air gap is left between the sections.
- Success Criteria – Ability to re-launch and propagate light on the subsequent fiber section. If this is not possible, a different method of sampling the soil gas via fiber will likely be necessary.
- Decision Point – Multispectral imager prototype field test results
- Success Criteria – Spatial resolution and spectral performance will be tested and NDVI or other image processing will be compared to commercial instruments.

Task 5.0 – Validation of Near-surface CO₂ Detection Techniques and Transport Models

- Decision Point – Many personnel – hours are spent by multiple institutions in the field experiment. Successful preparation / re-installation of field infrastructure must occur before conducting field experiment.
- Success Criteria – Packer system must inflate and hold pressure, mass flow control system must be functioning.

Technical Status

- Focus the remaining slides, logically walking through the project. Focus on telling the story of your project and highlighting the key points as described in the Presentation Guidelines
- When providing graphs or a table of results from testing or systems analyses, also indicate the baseline or targets that need to be met in order to achieve the project and program goals.

Presentation Outline

- Computational tool development
- Laboratory studies to understand subsurface CO₂ behavior
- Analog studies to inform risk analysis
- Near surface detection technologies / testing
- Mitigation method development

TOUGHREACT Version 2.0

Computers & Geosciences 37 (2011) 763–774



Contents lists available at ScienceDirect

Computers & Geosciences

journal homepage: www.elsevier.com/locate/cageo



TOUGHREACT Version 2.0: A simulator for subsurface reactive transport under non-isothermal multiphase flow conditions

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ARTICLE INFO

Article history:

Received 12 April 2010

Received in revised form

17 August 2010

Accepted 5 October 2010

Available online 18 November 2010

Keywords:

Multi-phase flow

Reactive transport

TOUGHREACT

CO₂ geological storage

Environmental remediation

Nuclear waste geological disposal

ABSTRACT

TOUGHREACT is a numerical simulation program for chemically reactive non-isothermal flows of multiphase fluids in porous and fractured media, and was developed by introducing reactive chemistry into the multiphase fluid and heat flow simulator TOUGH2 V2. The first version of TOUGHREACT was released to the public through the U.S. Department of Energy's Energy Science and Technology Software Center (ESTSC) in August 2004. It is among the most frequently requested of ESTSC's codes. The code has been widely used for studies in CO₂ geological sequestration, nuclear waste isolation, geothermal energy development, environmental remediation, and increasingly for petroleum applications. Over the past several years, many new capabilities have been developed, which were incorporated into Version 2 of TOUGHREACT. Major additions and improvements in Version 2 are discussed here, and two application examples are presented: (1) long-term fate of injected CO₂ in a storage reservoir and (2) biogeochemical cycling of metals in mining-impacted lake sediments.

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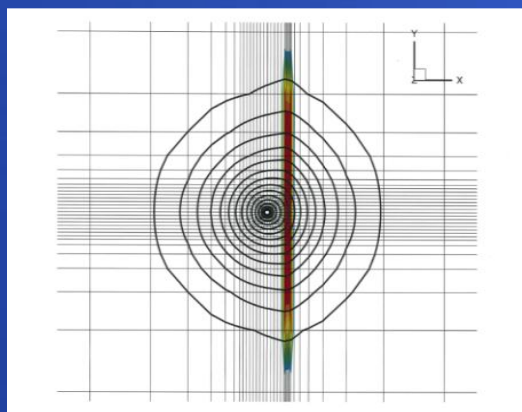
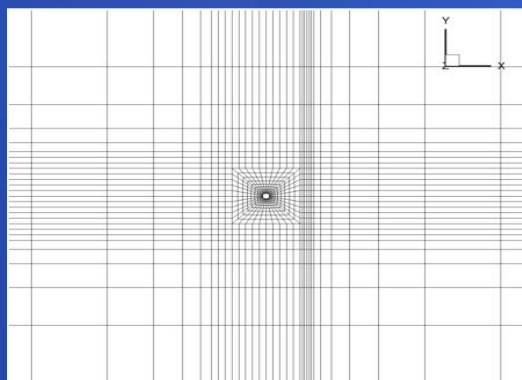
Development of numerical models for simulating coupled fluid-flow and stress effects

- Geomechanical impacts of large-scale injection during CO₂ storage operations is one of the critical issues in ensuring safe operations and long-term reliability of geologic CO₂ sequestration sites
- We have developed capabilities in LANL's FEHM reservoir simulator to model complex, **coupled non-isothermal, multi-phase flow and geomechanical processes**:
 - **Non-linear elasticity**: elastic moduli as functions of temperature, pressure, and stress
 - **Stress-dependant permeability models** : Non-linear, orders-of-magnitude permeability changes, explicitly or Implicitly coupled .
 - **Wellbore cement failure**: interface evolution due to geomechanical effects
 - **Plastic deformation**

Examples demonstrating new, complex fluid-flow and stress modeling capabilities in FEHM

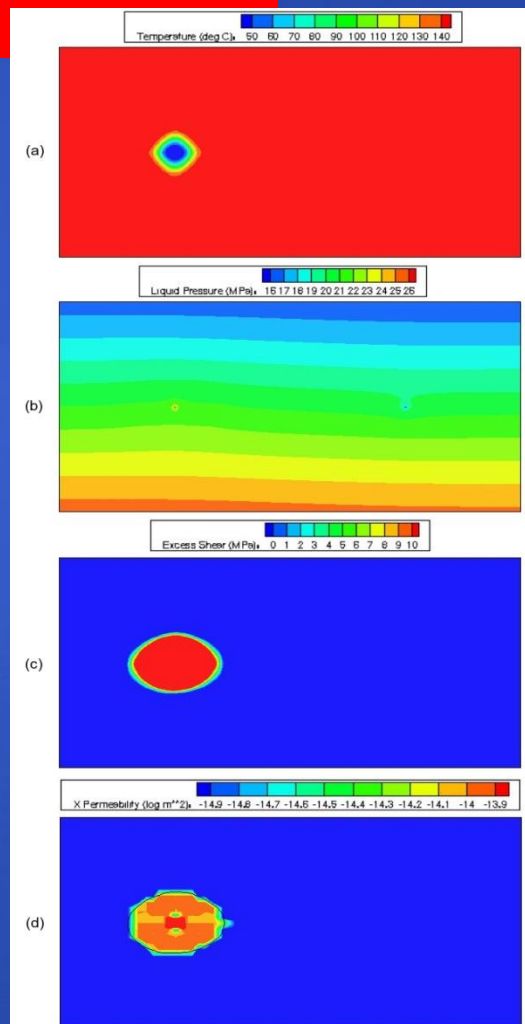
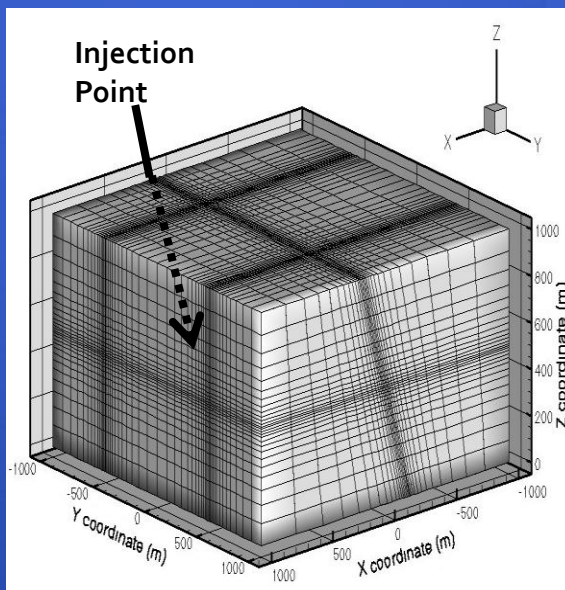
Simulation of change in the permeability in a fault due to injection in a nearby wellbore

Permeability as a function of change in normal stress



Simulation of change in permeability in an inclined fault due to injection

- Non-orthogonal grid
- Thermal effects
- Mohr-Coulomb failure
- Permeability as a function of shear stress



Comparison of silica/calcite wettability in the brine-scCO₂ and brine-N₂ systems

(Tim Kneafsey, Dmitriy Silin)

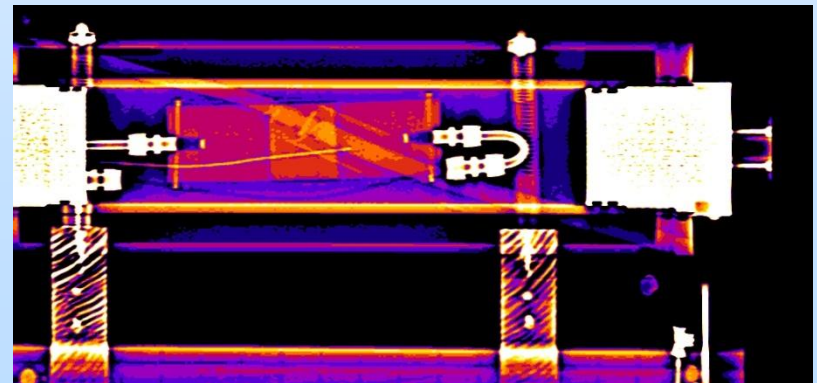
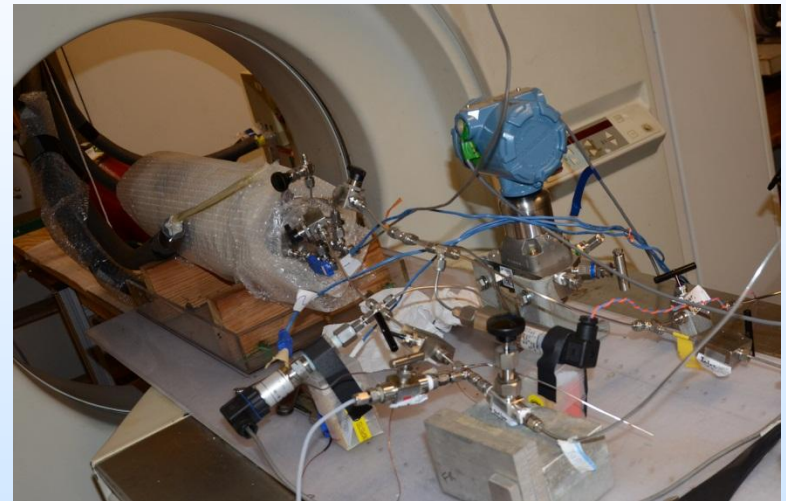
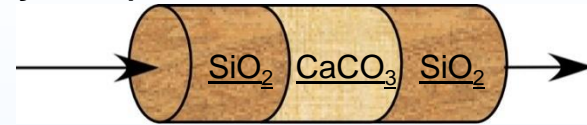


Objective

- Visualize/analyze wettability differences between coarse silica and fine calcite sand in scCO₂-brine system

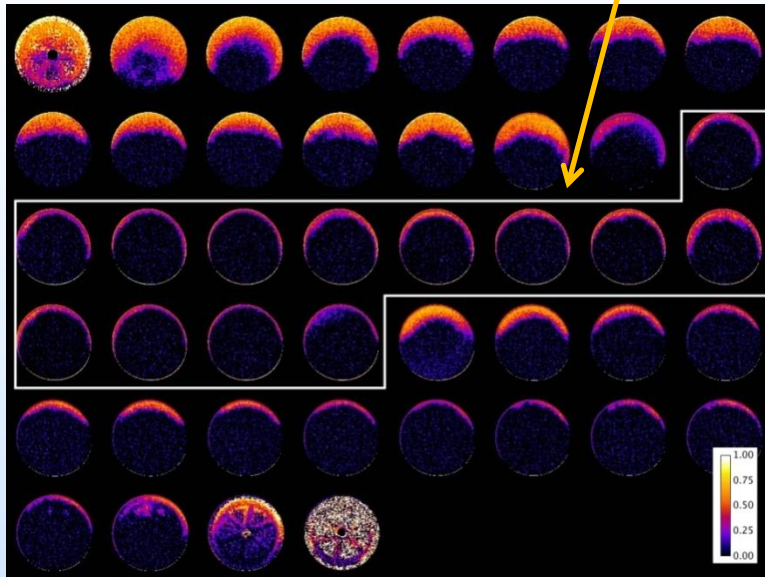
Approach

- Flow N₂ (for comparison) and scCO₂ through fine, brine-saturated sands
- Flow brine through sample after N₂, then scCO₂ until breakthrough (residual saturation)
- Monitor with X-ray computed tomography (CT)
- Image sand samples with microCT
- Apply Maximal Inscribed Spheres (MIS) model to compute characteristic curves
- Compare to experimental results

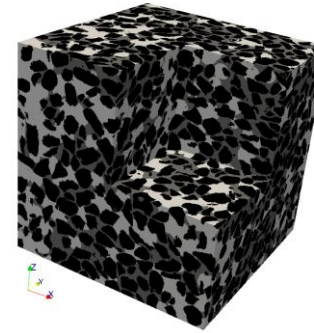


Experimental and Modeling Results

CT images of scCO_2 saturation in slices through composite domain (silica-calcite-silica) (calcite section is outlined by white line)

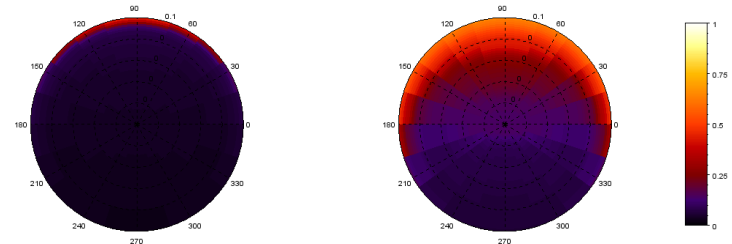


- Both N_2 and CO_2 flowed across sample top due to gravity
- Both N_2 and CO_2 flowed through a larger region of silica than calcite
- Neither N_2 or CO_2 penetrated deeply into calcite indicating strongly brine-wetting conditions



MicroCT imaged sand and calculated pore occupancy by MIS

Computed scCO_2 saturation using MIS computations for 0 and 20 degree contact angles

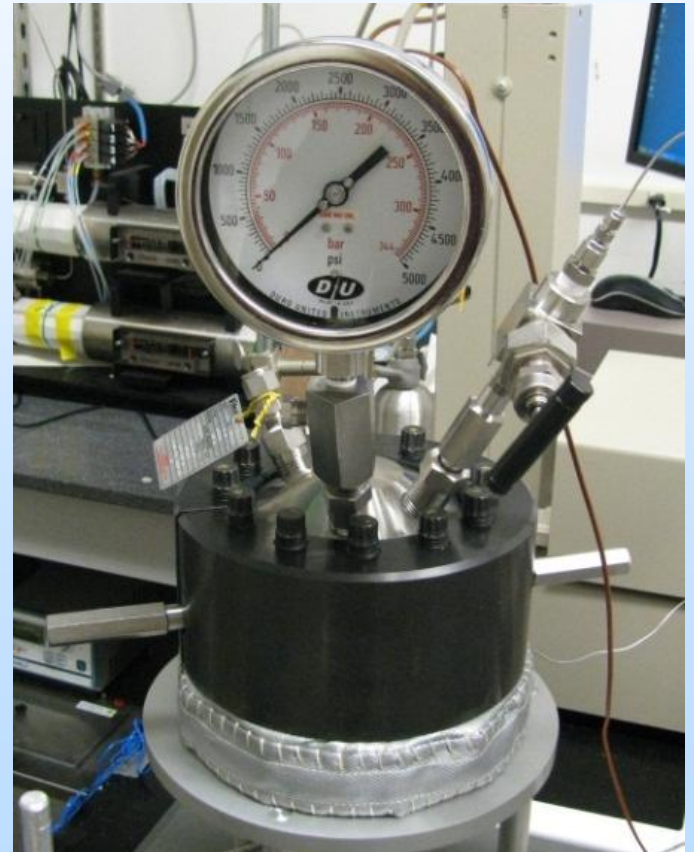
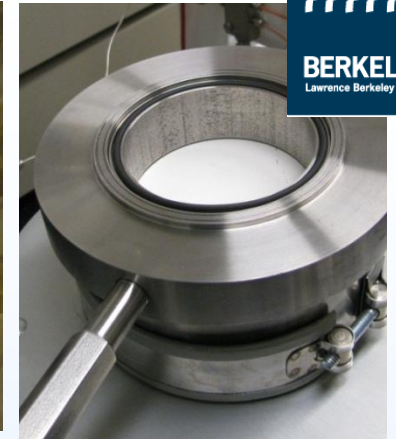


- Computations based on the MIS technique including contact angle indicate that both silica and calcite are brine-wetting, but calcite is strongly brine-wetting under the experiment conditions.

Capillary Pressure-Saturation Relations

(Jiamin Wan and Tetsu Tokunaga)

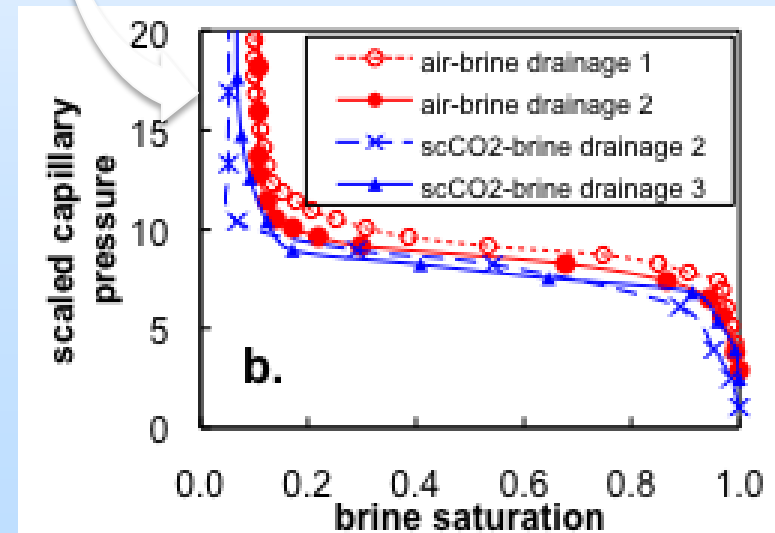
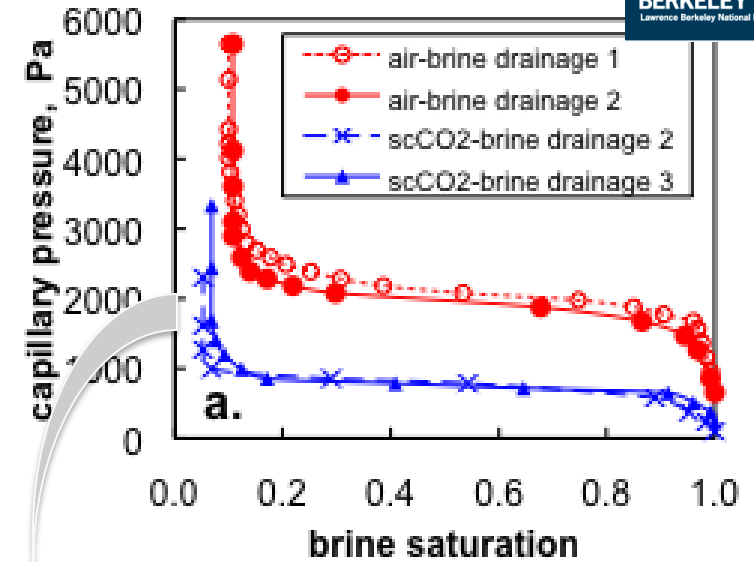
- Saturation-capillary pressure, $S(P_c)$, relations are needed to determine equilibrium of CO_2 -brine, relative permeability relations, flow, and residual trapping of CO_2 .
- Measurements are being done on well-characterized, uniform sands in order to quantitatively compare results with predictions based on capillary scaling models.
- Our experimental system is capable of measuring $S(P_c)$ relations on unconsolidated (sands) and consolidated (cores).
- Experiments have been conducted on air-water systems at atmospheric pressure and 20°C , and on scCO_2 -water(brine) systems at high pressure (8.5 to 12 MPa) and 45°C .



Example Results and Implications

- $S(P_c)$ relations for systems involving $scCO_2$ exhibit drainage at lower P_c , qualitatively consistent with expectations from low interfacial tensions of $scCO_2$ -water.
- Capillary scaling provides only approximate predictive capability in $scCO_2$ -brine systems.
- Alterations mineral surface wettability in $scCO_2$ /brine/mineral systems* are important in altering $S(P_c)$ behavior, and may contribute to more complex, larger-scale behavior of $scCO_2$ in geologic C sequestration.

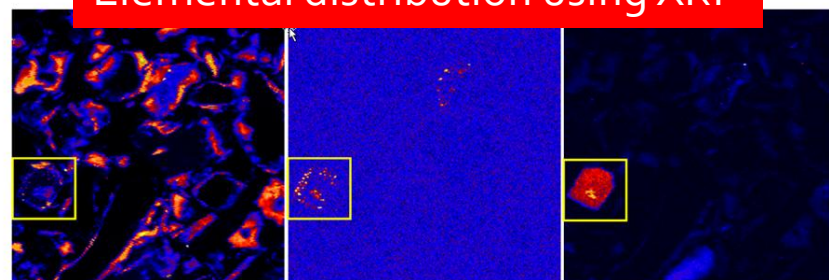
* Jung and Wan, 2012, Energy & Fuels (in press).



Characterization of trace-metal release due to CO₂ leakage in shallow aquifer

- Samples of rocks from Chimayo were characterized and exposed to CO₂ in laboratory experiments
- As, Pb and U were often found attached to Fe associated with clay
- Experiments show that Arsenic is quickly released as CO₂ is introduced to the system but slowly returns to background concentrations
 - Type II scavenging as defined by Smyth et al. (2006) could be an explanation

Elemental distribution using XRF

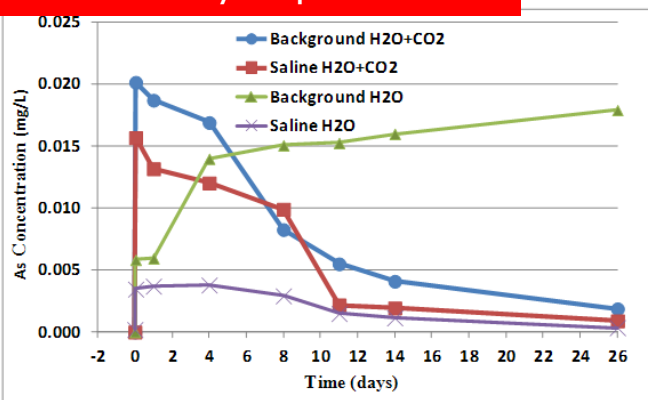


a) Iron

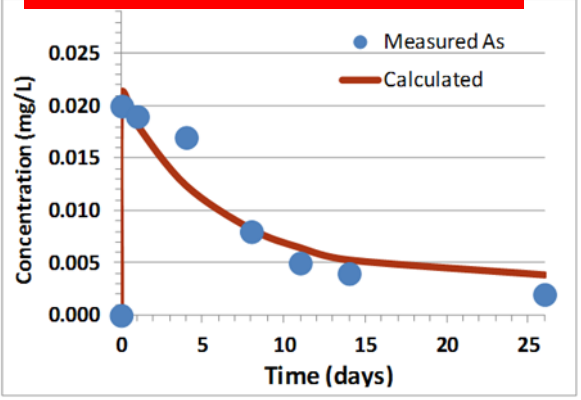
b) Arsenic

c) Uranium

Laboratory experiments



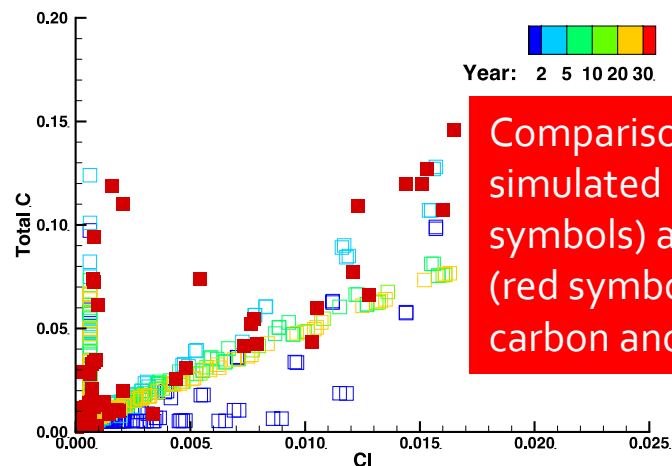
Geochemical modeling



- A geochemical model with sorption to iron-hydroxides on the clay was developed
- Calcite buffering and As sorption identified as processes controlling pH and As concentrations

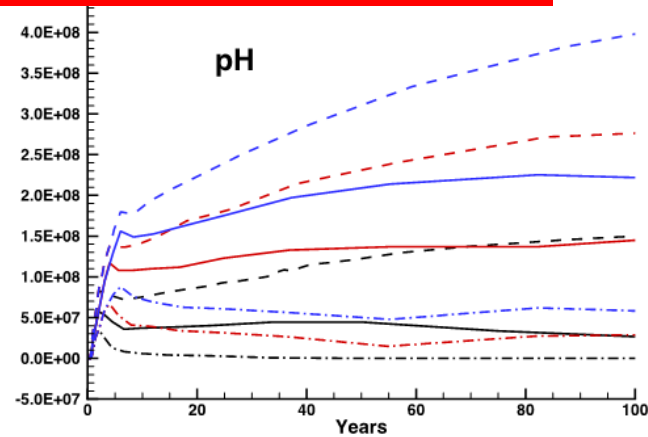
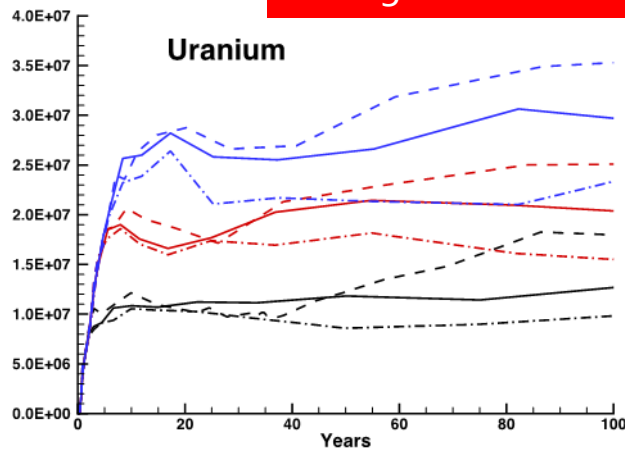
Prediction of dynamic evolution of geochemical impacts of CO₂ leakage

- A field-scale multi-phase, reactive transport model was developed and calibrated using data from the Chimayó natural analog site
- The model was used to constrain reactive-transport model parameters and to infer leakage rate along a fault
- Calibrated model was used to simulate CO₂/brine leakage scenario and to predict long-term geochemical interactions
- Results show very slow recovery after cessation of CO₂ leak
- Co-transport of saline water with CO₂ is more detrimental to shallow groundwater quality than in-situ metal mobilization



Comparison of simulated (open symbols) and measured (red symbols) total carbon and chloride

Predicted evolution of Uranium and pH post-CO₂ leakage





LLNL goals for ZERT II



- 1) Develop and validate models of historic natural gas migration and surface release using existing software tools. Can we replicate these historic events?

- 2) Investigate the methodologies and data analysis algorithms to use satellite data to monitor leakage from CO₂ sequestration sites.





We routinely use codes to predict movement of gas and fluids prior to conducting field tests



- We developed a 3D gas migration model built on a realistic site geological model of the aquifer gas storage reservoir at the Leroy natural gas storage facility, which experienced uncontrolled gas leakage in the 1970s. The 3D model was validated by field pressure and inventory data. The simulated methane distribution was analyzed to evaluate the leakage pathways, which are highly relevant to other subsurface applications, such as CO₂ storage. Our results indicate that a discrete (rather than diffuse) leakage pathway is required and that fault leakage is a likely explanation for the observed gas leakage, although the possibility of wellbore leakage has not been entirely ruled out and should be considered in future work.





Satellite technology for monitoring CO₂



- During FY11 we investigated the methodologies and data analysis algorithms to use satellite data to monitor leakage from CO₂ sequestration sites.

- The technical work pursued three paths:
 - Use of currently available satellite data (e.g., GOSAT and Sciamachy) to develop the data analysis techniques and data acquisition CONOPS.
 - Analytical work to develop models for the minimum detectable leakage rate as a function of area of leakage, wind speed, wind direction, and observation time.





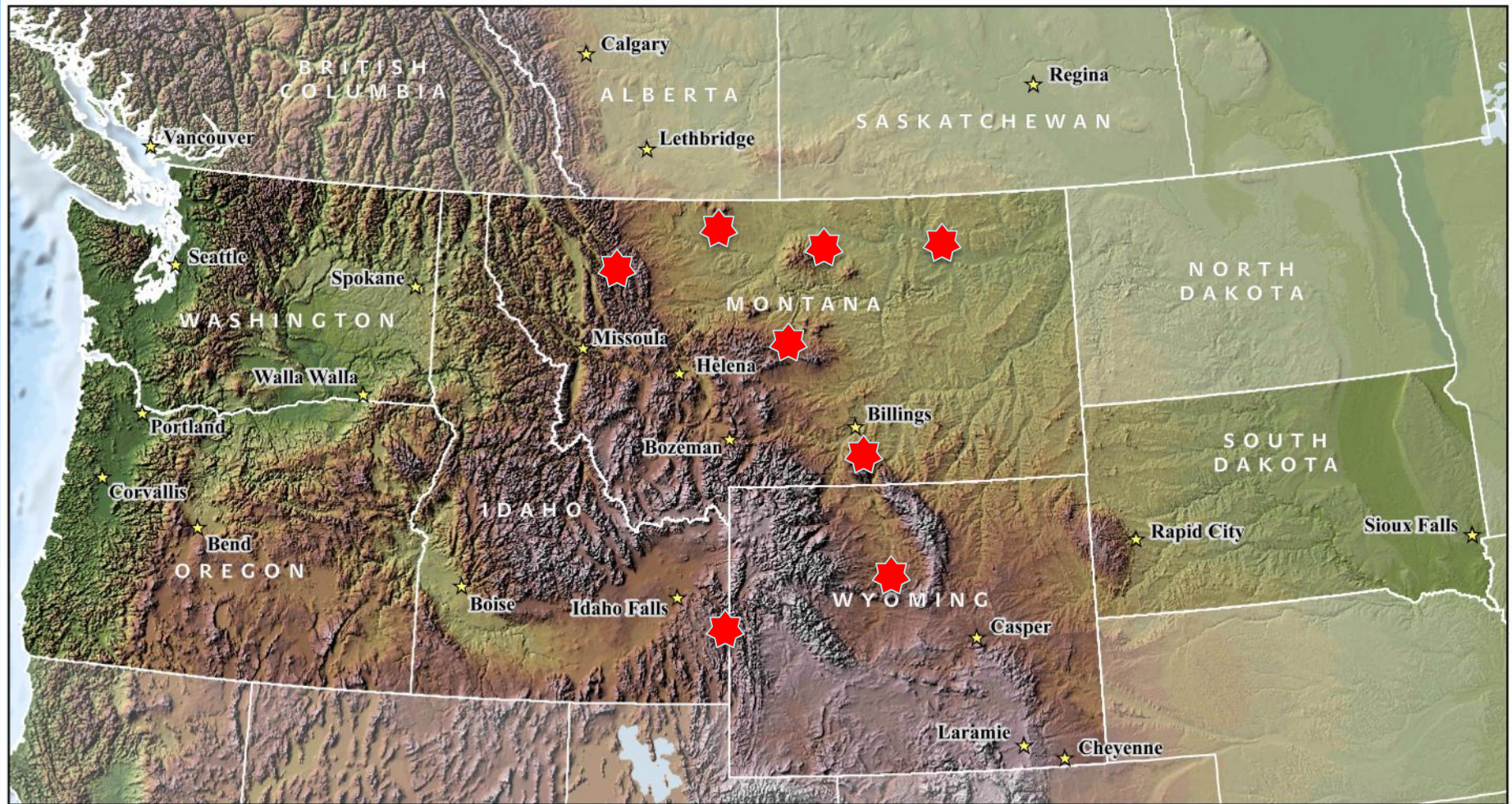
Collaborators and Participants



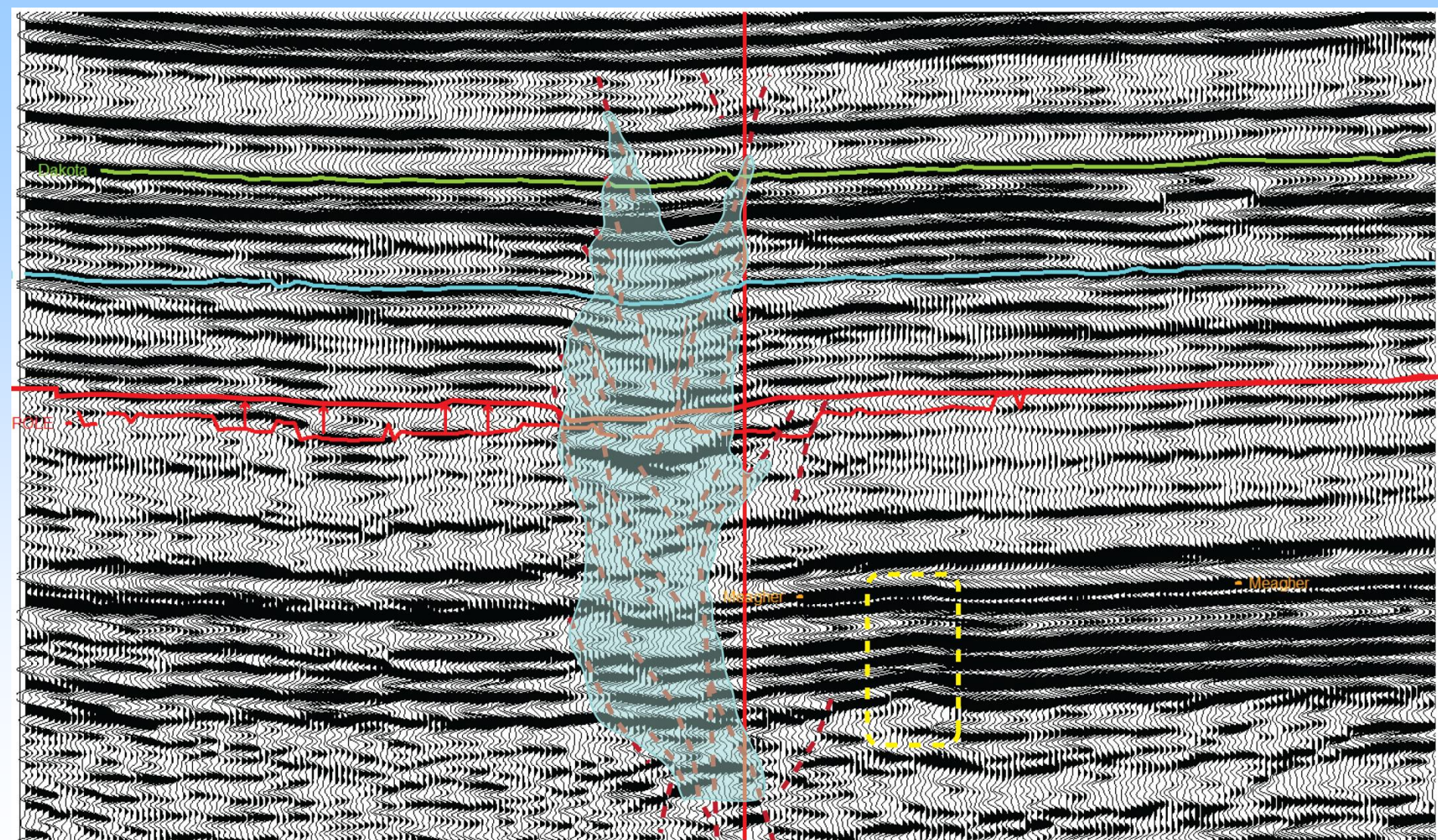
- UC Santa Cruz was subcontracted to perform the bulk of the work, led by Eli Silver who is the founding Director of the UCSC Center for Remote Sensing.
- Technical direction and data analysis was performed by LLNL staff experienced in satellite remote sensing (John Henderson).
- Sam Vigil, Professor of Environmental Engineering, California Polytechnic State University, also collaborated with LLNL and UCSC.

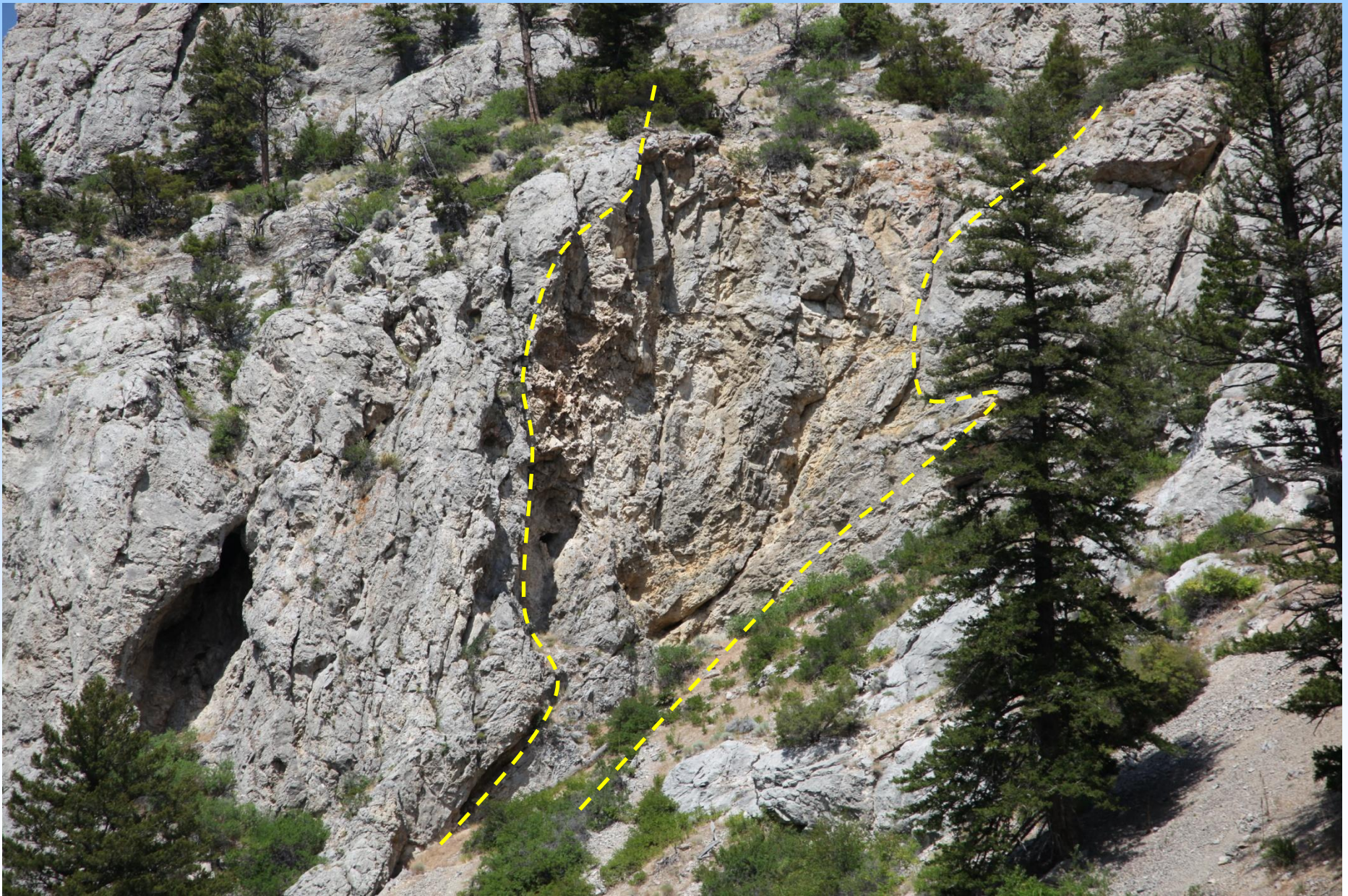


Ongoing Hydrothermal Research Projects

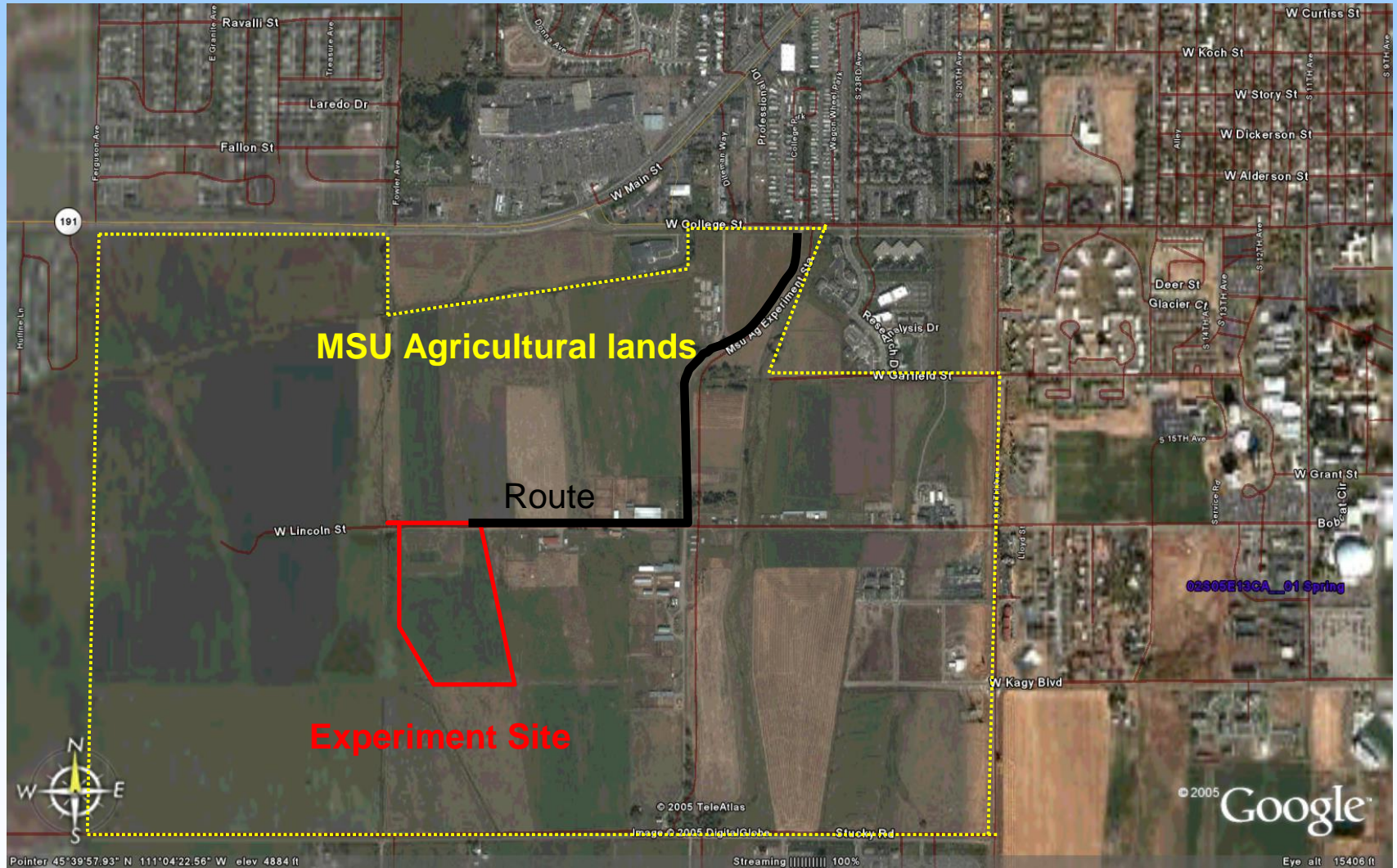


“Sag” in Reflection Seismic Data



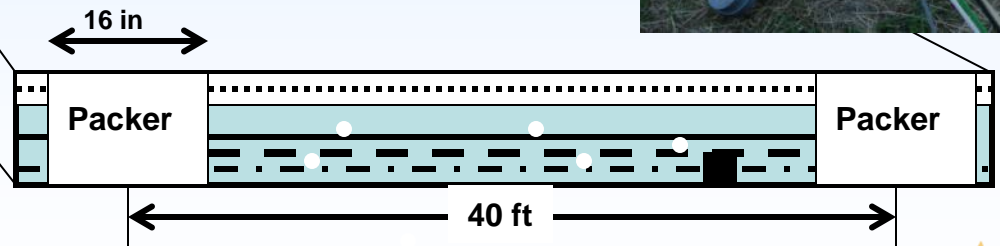
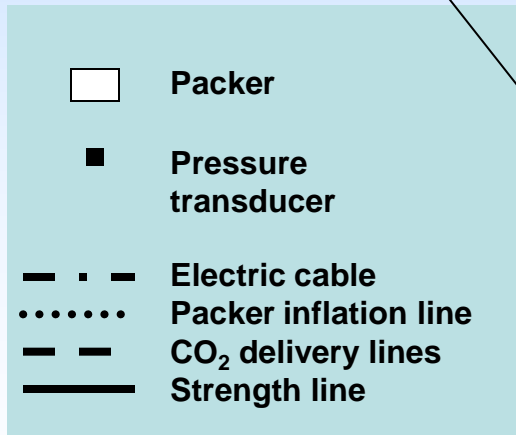
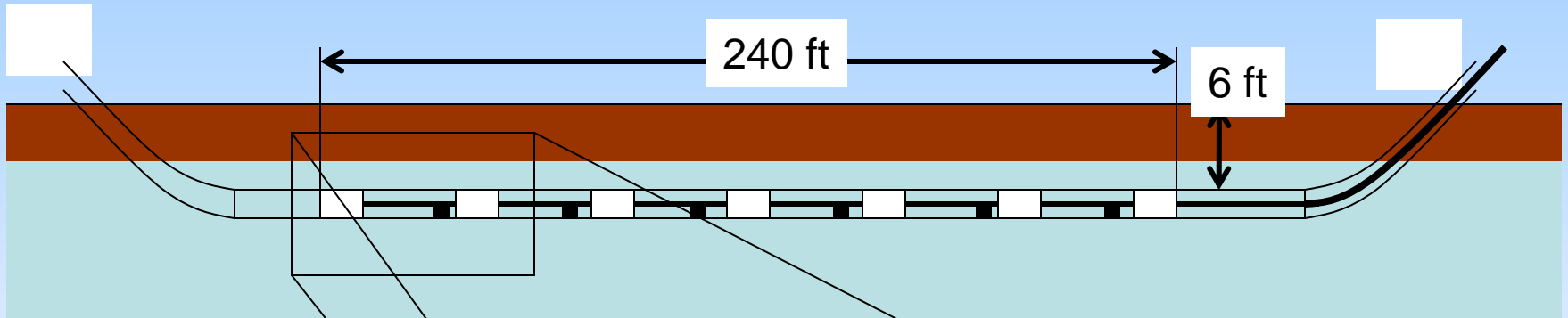


Field Test Facility



Horizontal Well Installation

Ray Solbau, Sally Benson

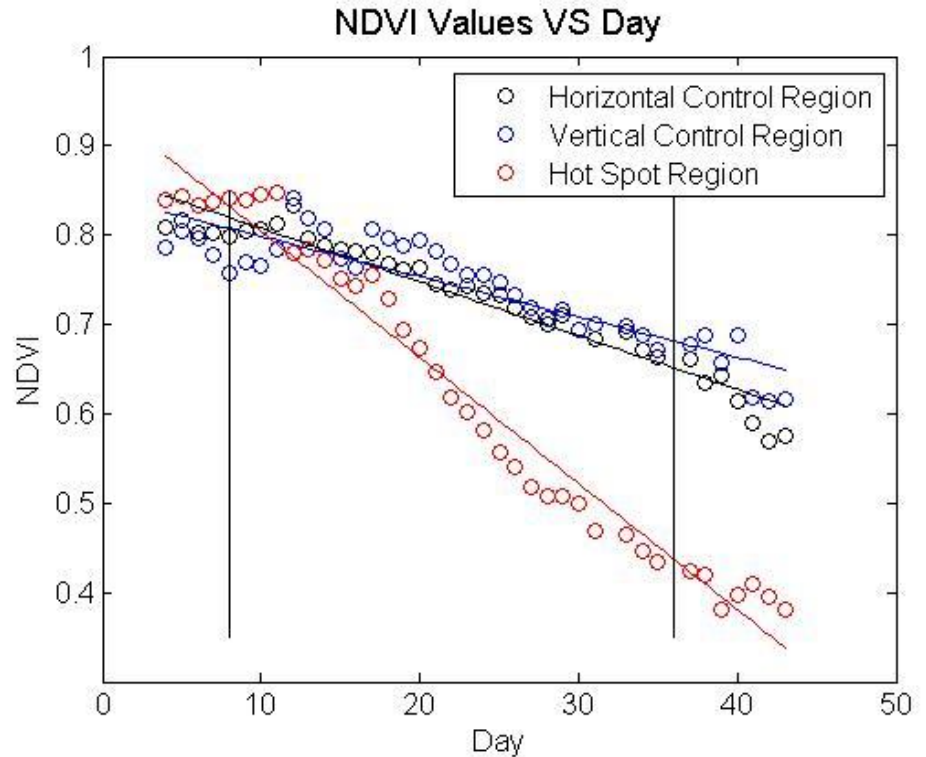


Multi-spectral imaging for detecting CO₂ leaks

J. Shaw



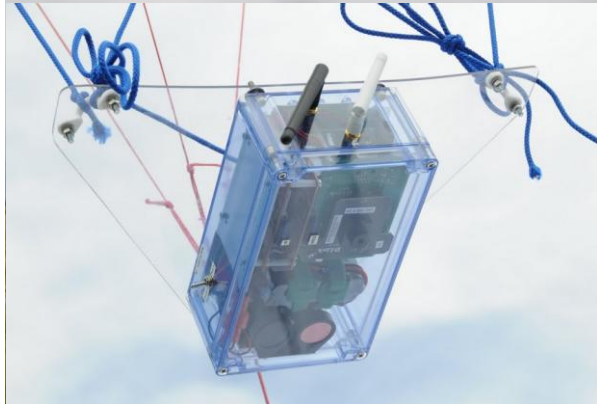
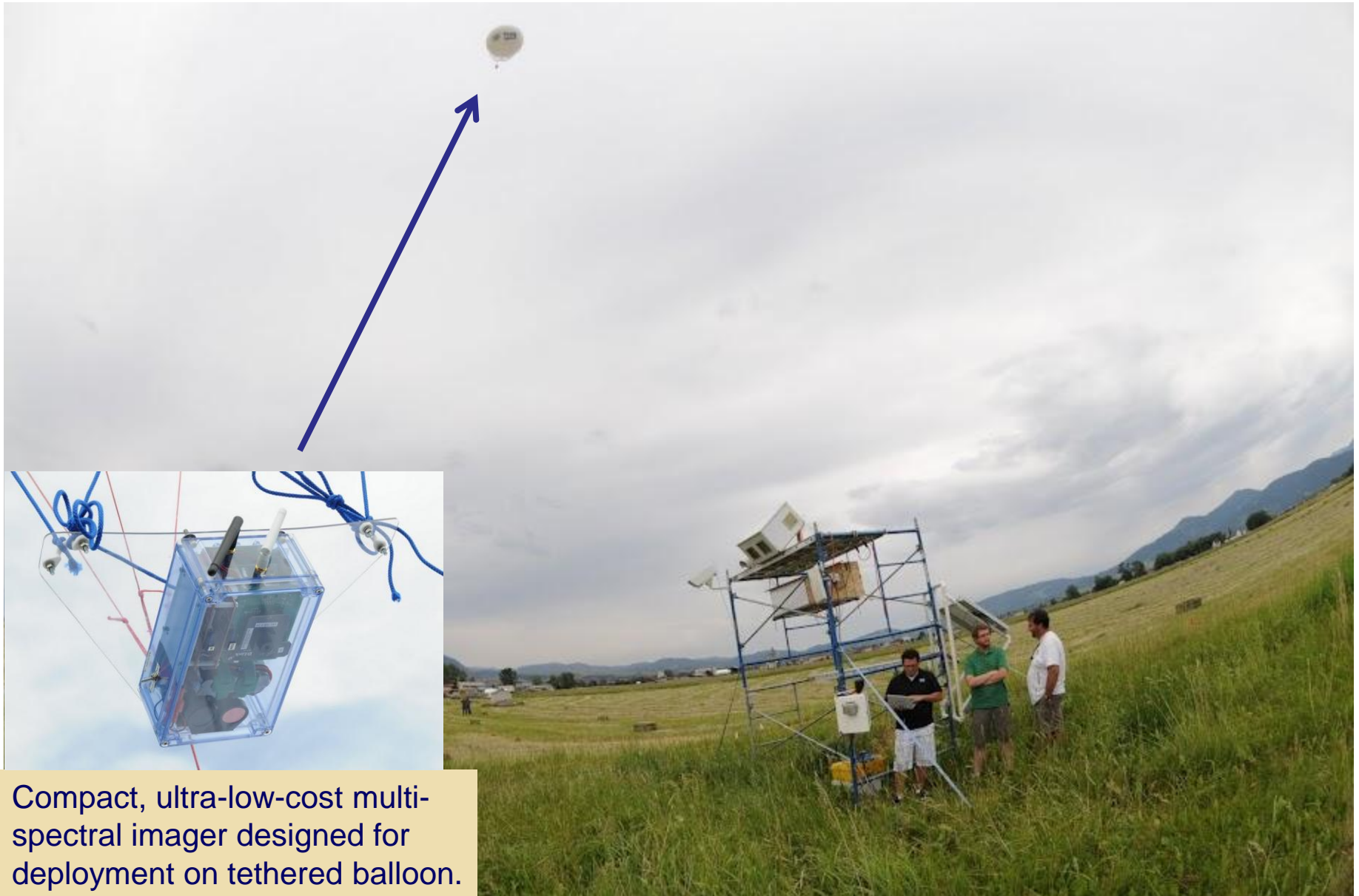
Multispectral imagers used to detect plant stress caused by CO₂ leaking from underground.



Time-series plot showing that the CO₂-affected plant health decays faster over time than the control region. This plot shows Normalized Difference Vegetation Index (NDVI), found from NIR and red reflectances as $(\text{NIR} - \text{red}) / (\text{NIR} + \text{red})$

Tethered balloon multispectral imaging at ZERT

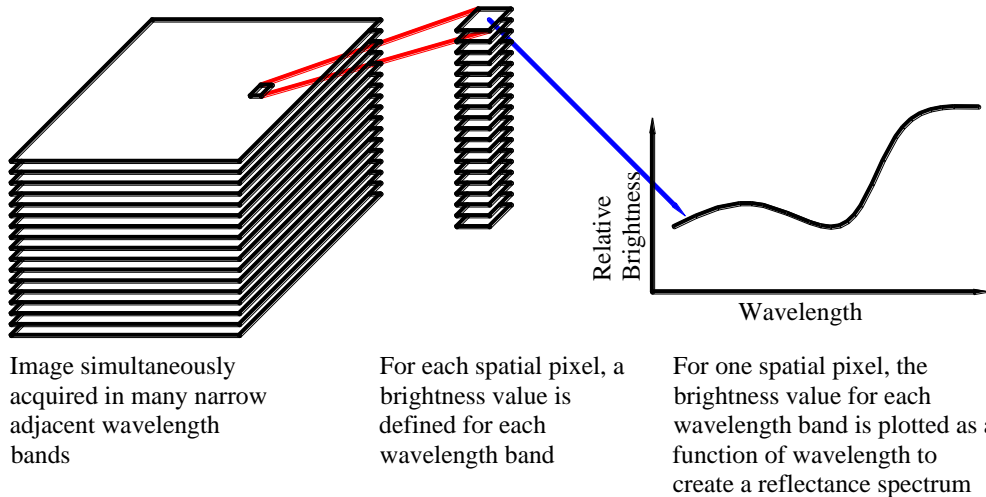
J. Shaw



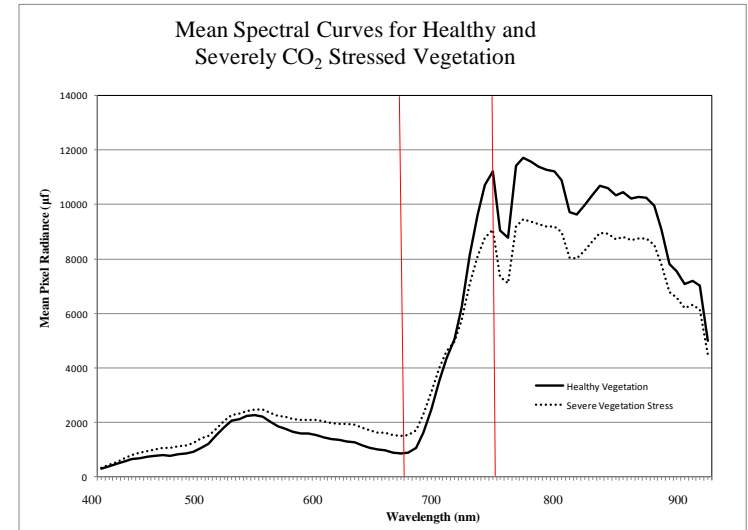
Compact, ultra-low-cost multi-spectral imager designed for deployment on tethered balloon.

Hyperspectral Aerial Detection

K. Repasky



For each pixel in the image, a reflectance spectra – amount of light reflected as a function of wavelength -- is generated



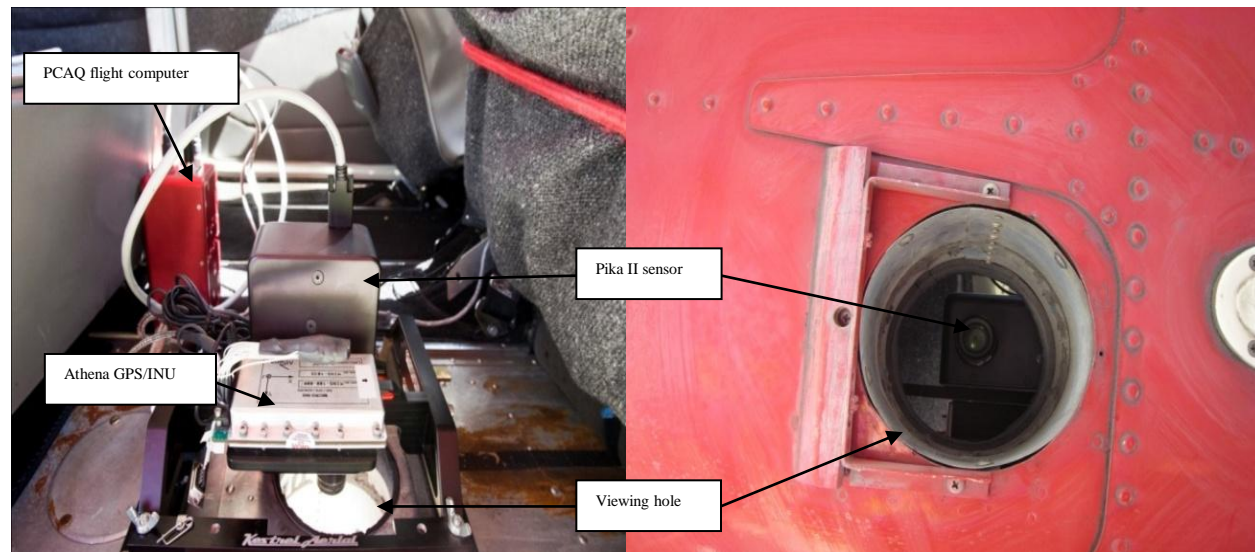
Stressed vegetation can be detected by detected using subtle changes in the reflectance spectra resulting from plant physiology

Hyperspectral Aerial Detection

K. Repasky



Flight based hyperspectral imaging allows large area monitoring needed for carbon sequestration sites



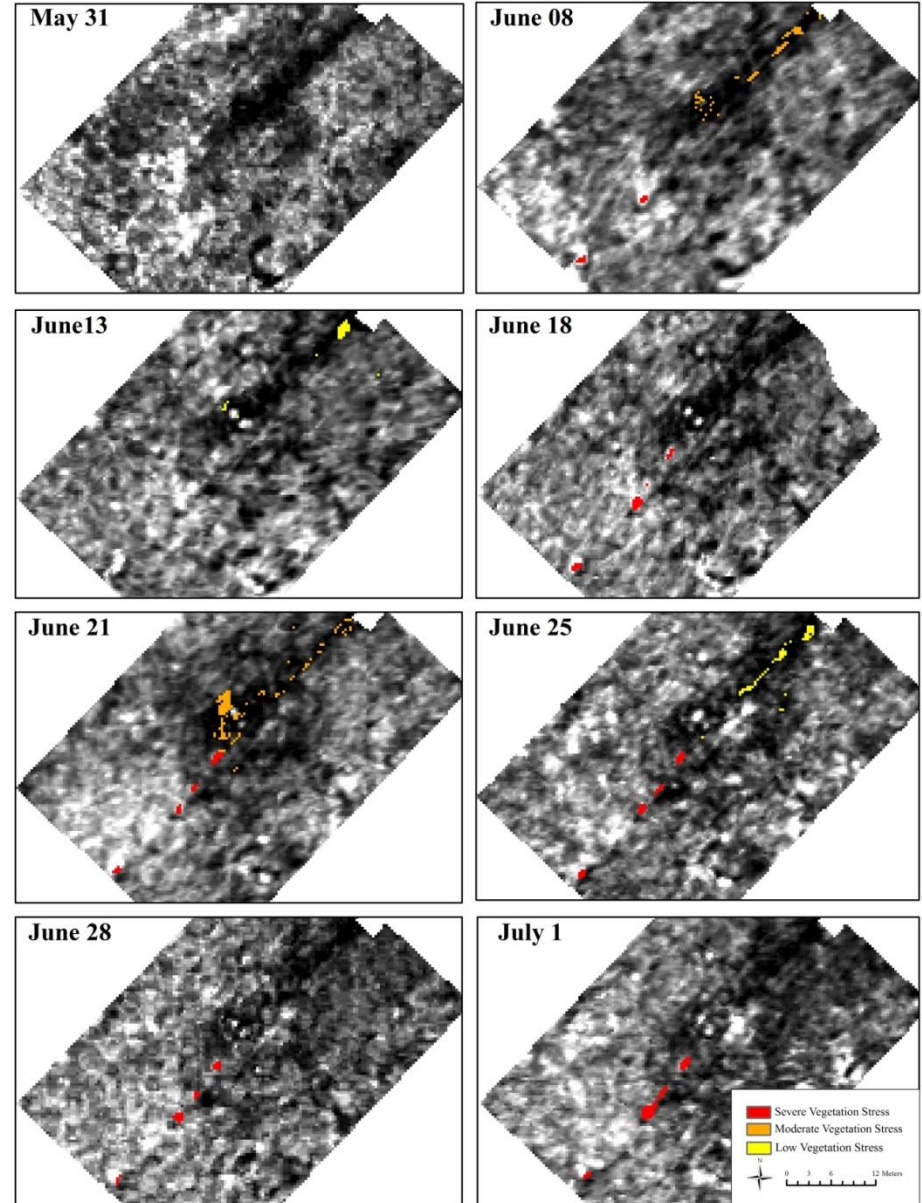
K. Repasky



Aerial view of the ZERT field site

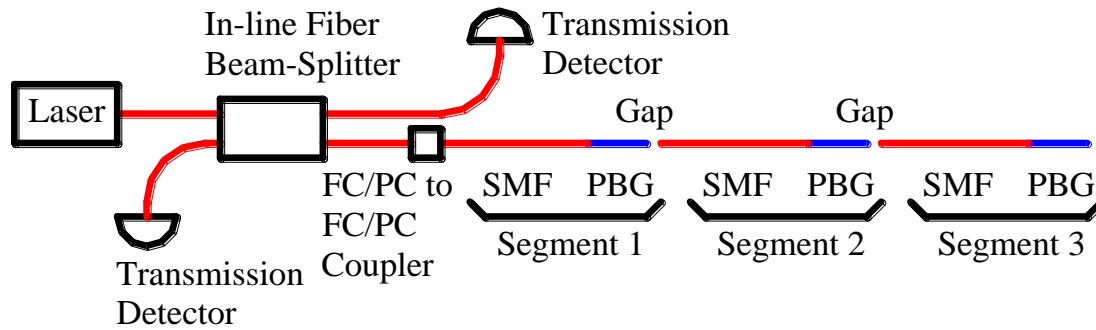
Evolution of the vegetation stress over the course of a month long sub-surface release at the ZERT field site.

The stress vegetation correlates with chamber measurements of carbon dioxide providing a validation of this method.



Inline Fiber Sensor

K. Repasky

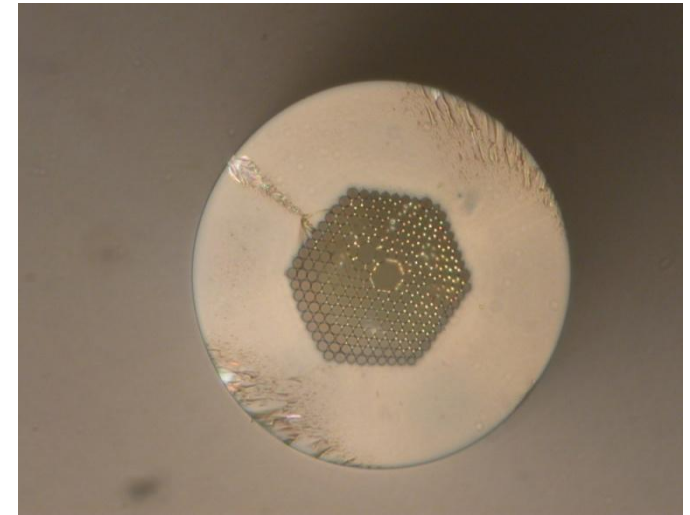


The inline fiber sensor uses a series of segmented photonic bandgap (PBG) fiber in series to for a inline fiber sensor array.

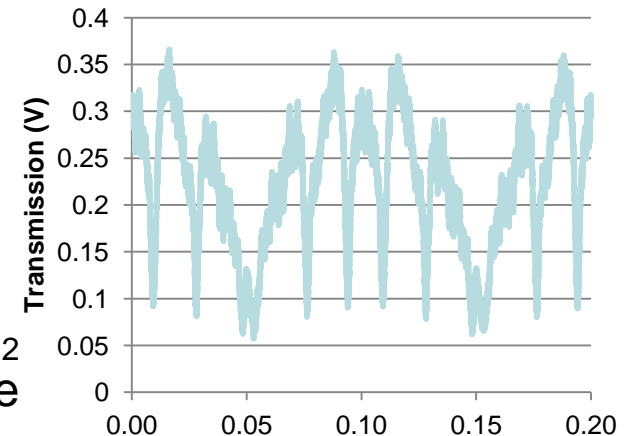
Each segment is addressed using time of flight of the laser pulse.

CO₂ diffuses into the PBG fiber to allow spectroscopic measurements of CO₂ concetration.

Initial un-normalized CO₂ measurements made using one segment of the inline fiber sensor.



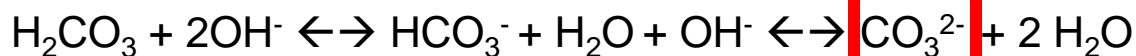
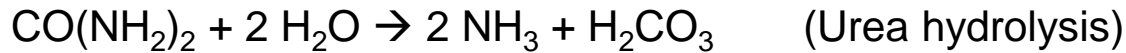
The PBG fiber allows interaction of the laser light and CO₂ in the hollow core.





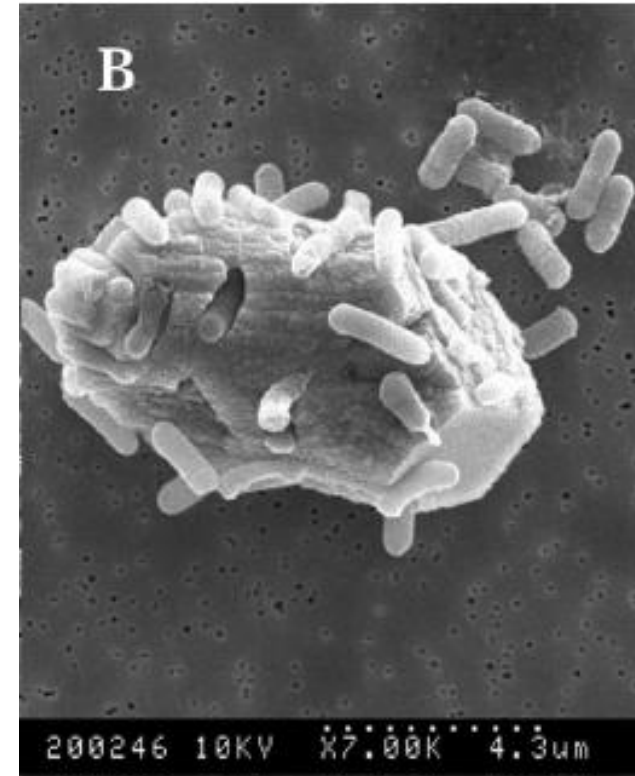
Cunningham, Gerlach

+ pH and alkalinity (increase in OH⁻ and HCO₃⁻)
increase SATURATION STATE OF CALCITE



Model ureolytic organism: *Sporosarcina pasteurii*

Ureolysis is only one possible way to
manipulate the saturation state of
carbonates



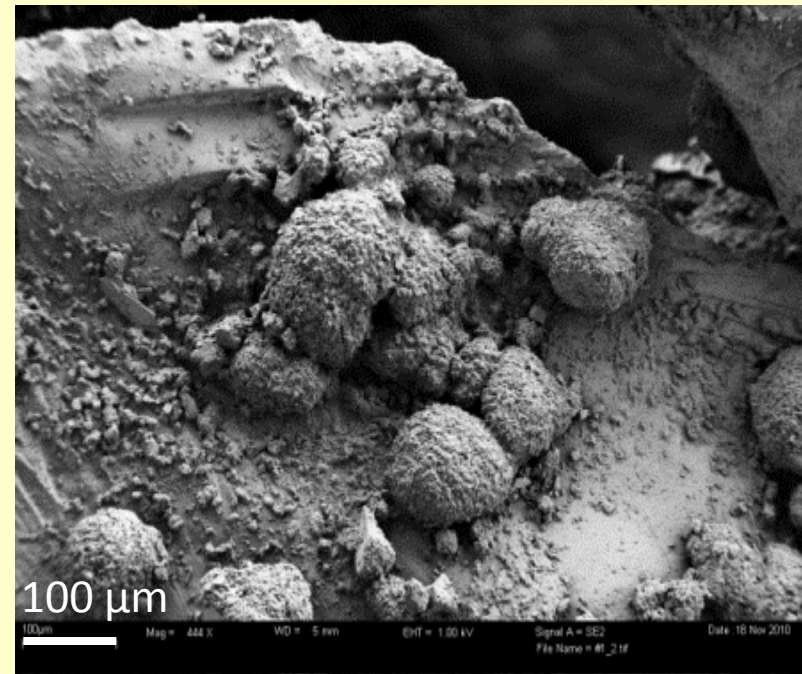
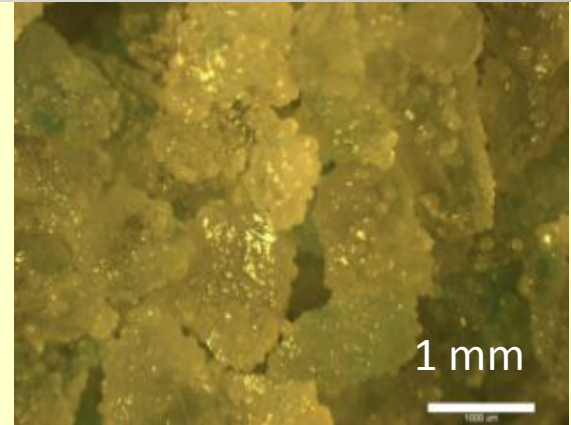
Mitchell, AC and Ferris, FG (2006).
Geomicrobiology Journal, 23, 213-226.

Mitchell, AC. and Ferris, FG. (2006)
Environmental Science and Technology,
40, 1008-1014.

Mitchell, AC. and Ferris FG. (2005)
Geochimica Et Cosmochimica Acta, 69,
4199-4210.

Pulse-Flow Calcite Precipitation in 2ft Sand Columns

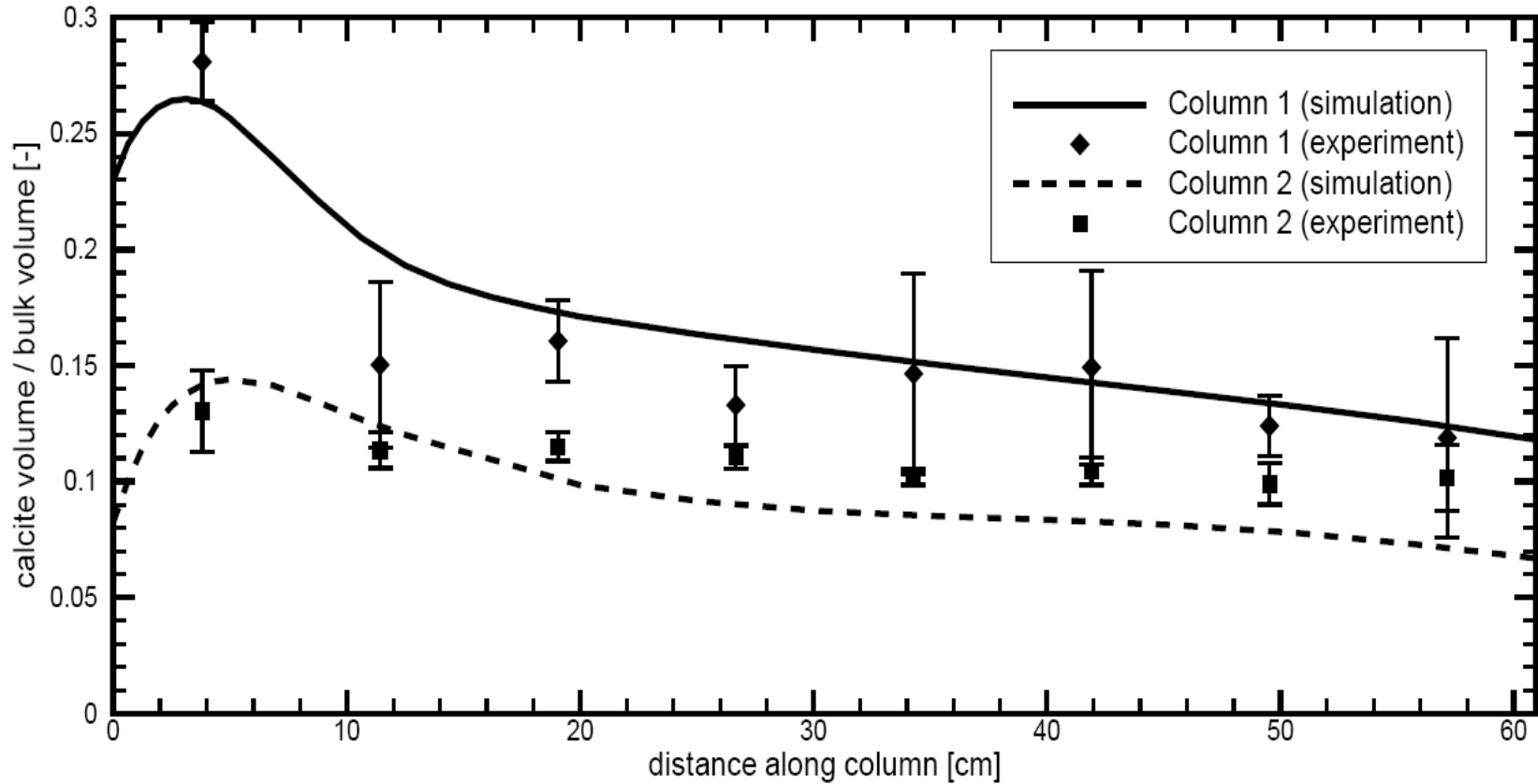
Cunningham, Gerlach



A. Phillips, J. Stringam,

Pulse-Flow Calcite Precipitation in 2ft Sand Columns

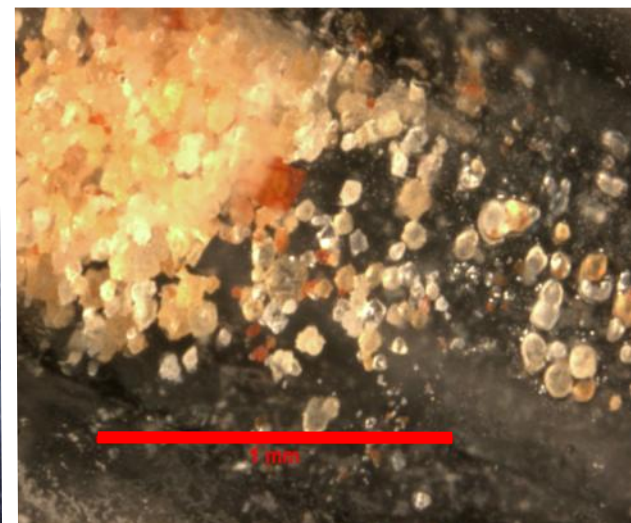
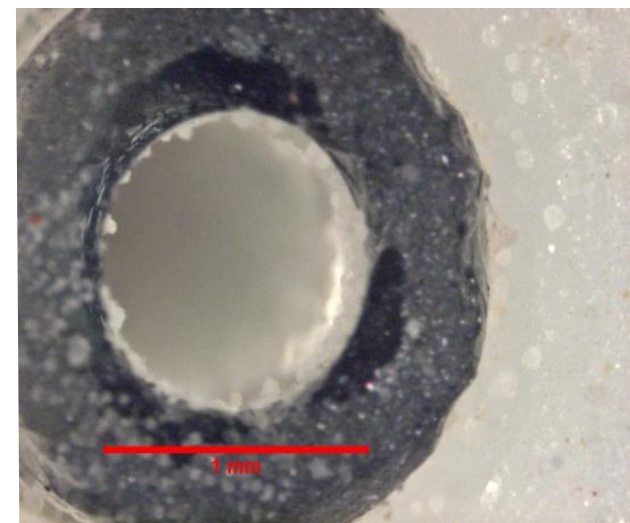
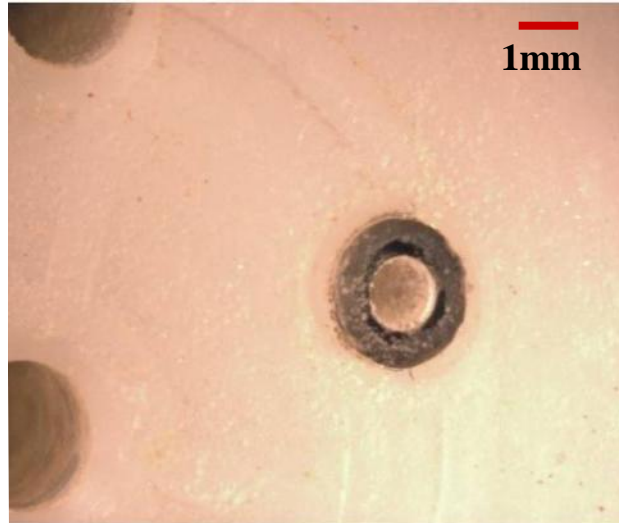
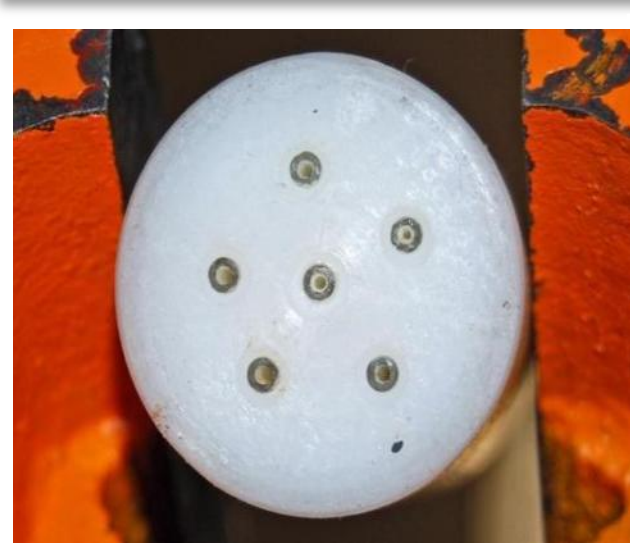
Cunningham, Gerlach



- 1) **CMM+:** Rich media (3 g L⁻¹ nutrient broth), Ca (13.6 g L⁻¹; 0.33 M), Urea (20 g L⁻¹; 0.33M)
- 2) **CMM- :** Rich media (3 g L⁻¹ nutrient broth), Urea (20 g L⁻¹; 0.33M)
- 3) **CMM=:** Rich media (3 g L⁻¹ nutrient broth)

A. EBIGBO, ET AL. IN PRESS. MODELING MICROBIALLY INDUCED CARBONATE MINERAL PRECIPITATION IN POROUS MEDIA

Ureolysis-Driven CaCO_3 Formation at High Pressure under Pulse-Flow Conditions

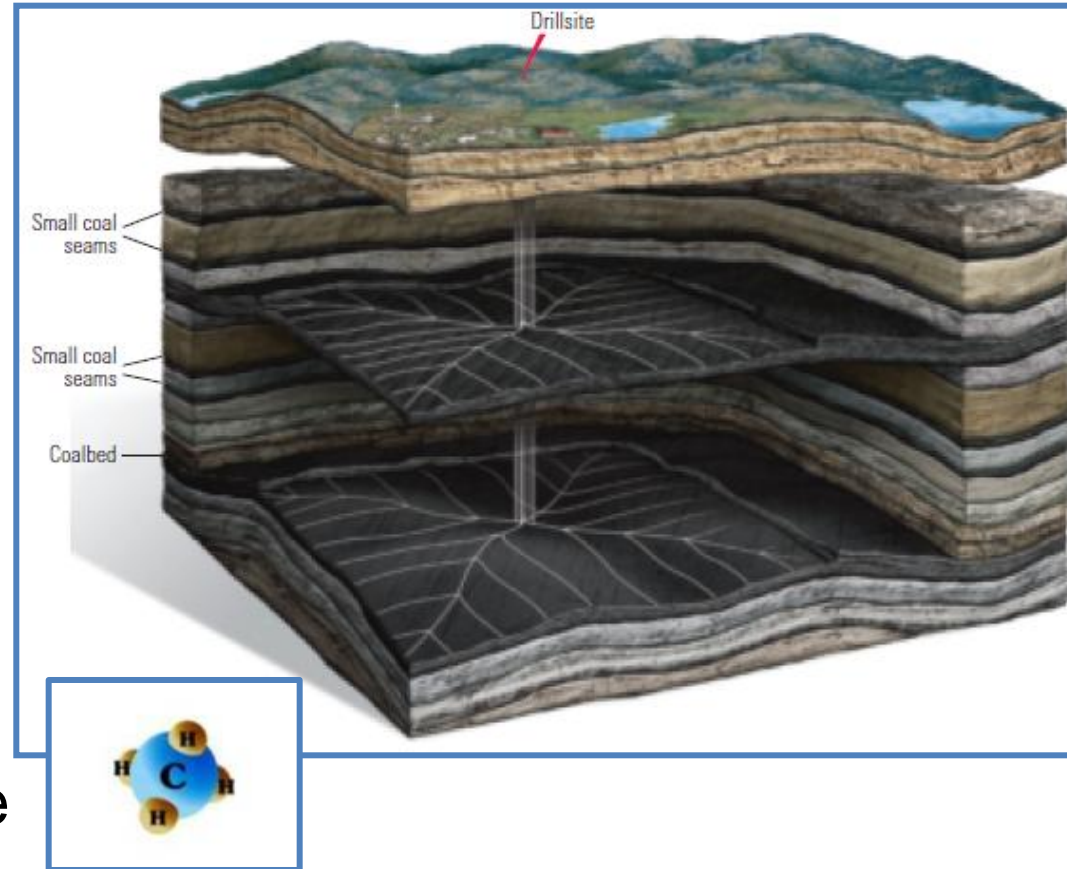


Logan Schultz

Sustainable microbial coal bed methane production

Methane can be formed through the biotransformation of organic matter (including coal and oil) by methane producing microorganisms (*Methanogens*).

By supplying appropriate nutrients to the coal & oil deposits microbial methane production can be enhanced and sustained over time



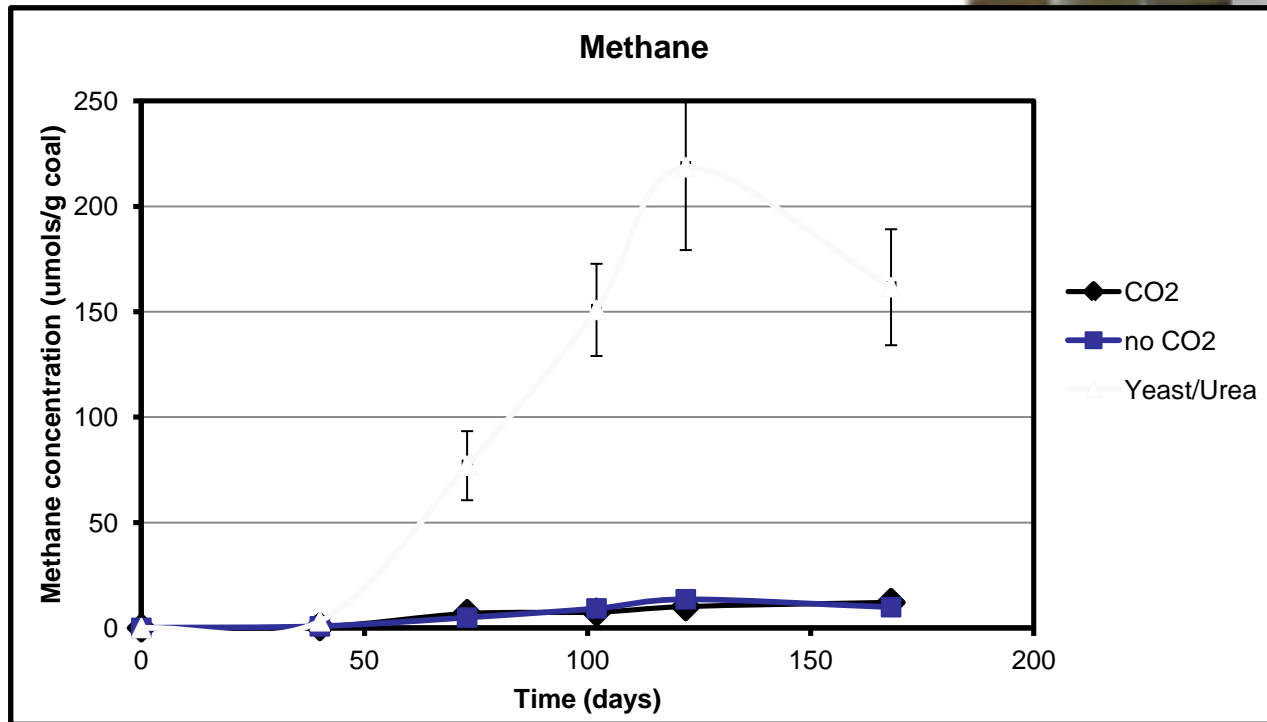
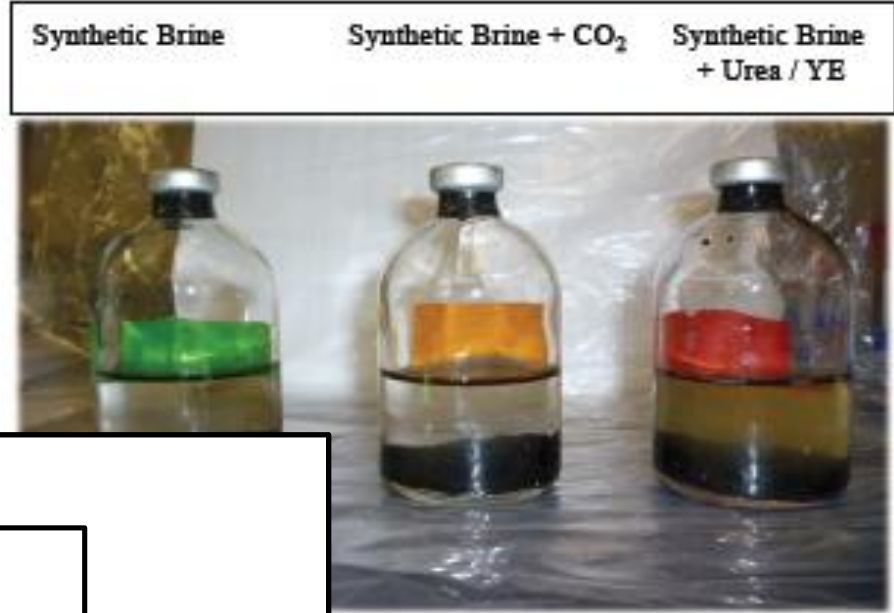
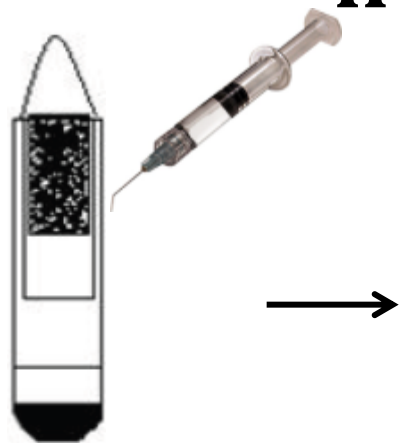
Sampling Powder River coal beds, October 2011

Conducted by USGS with MSU student participation



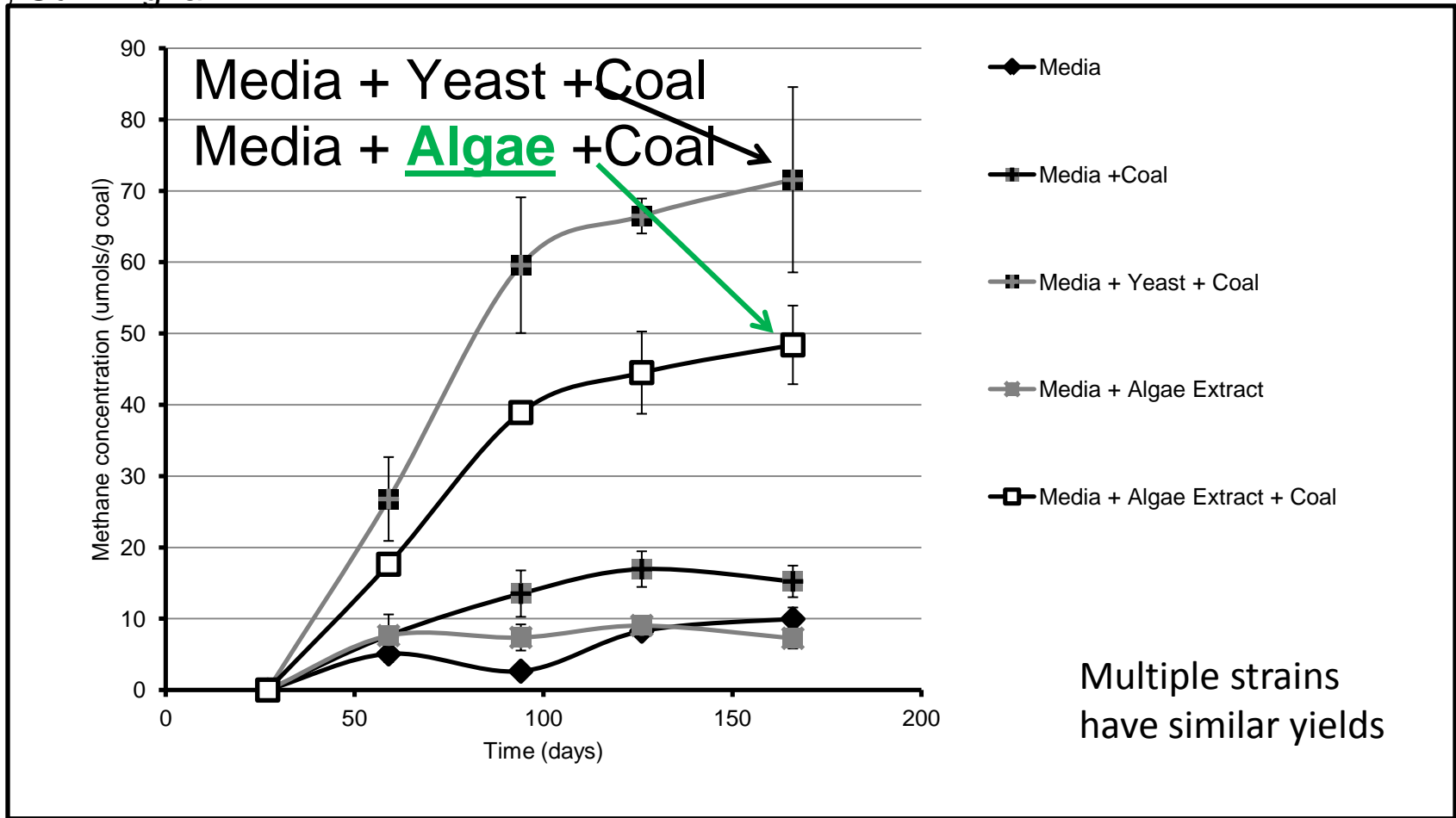
Biostimulation of methane production from coal

Fields, Cunningham

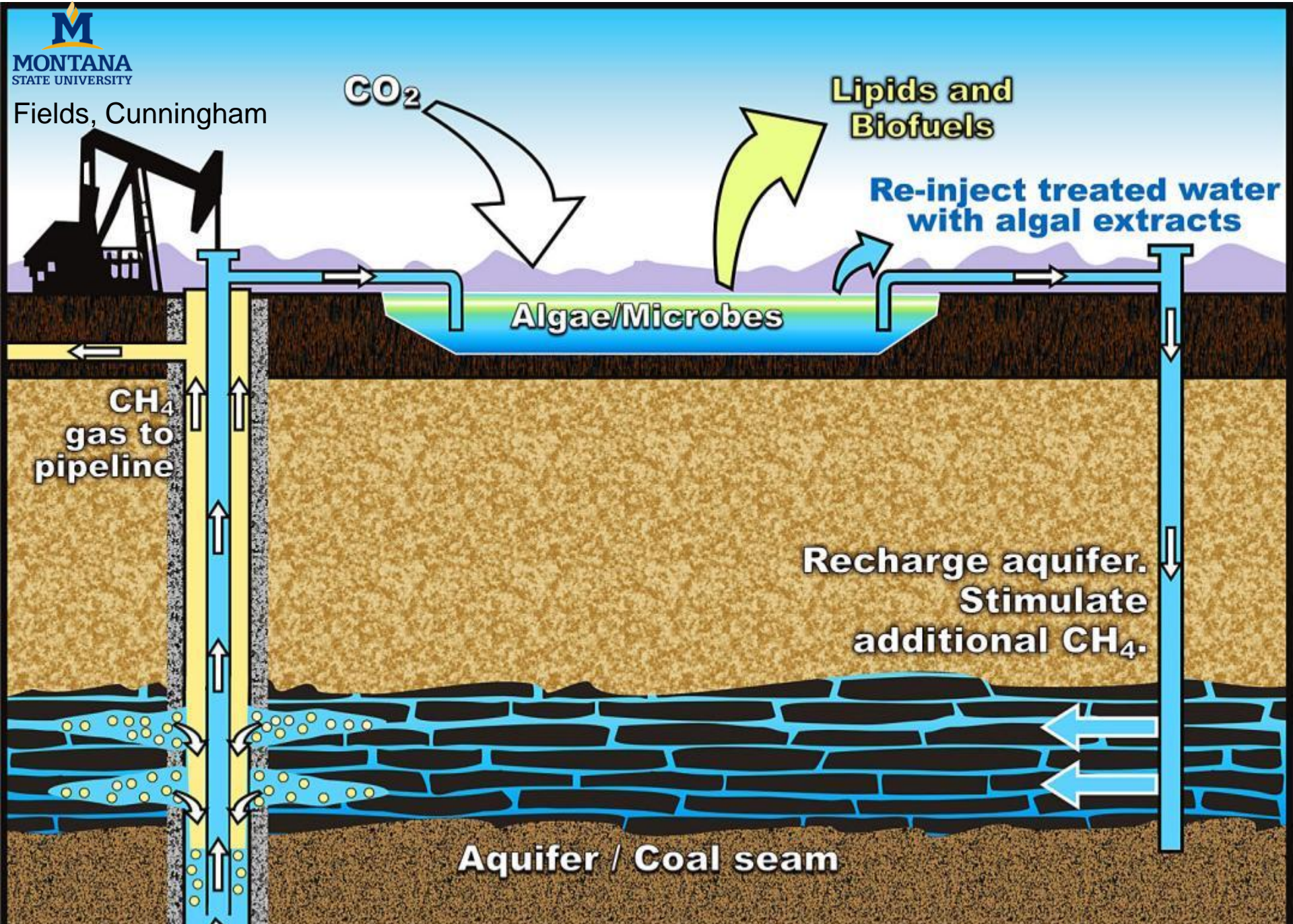


Algae enhanced methane production from coal

Fields, Cunningham



Elliott Barnhart: "In situ and enriched microbial community composition and function associated with coal bed methane from Powder River Basin coals"



Accomplishments to Date

- Modified two computational codes used for CO₂ simulations
- Studied multiple analogs to inform risk assessment
- Developed and performed initial field tests on three prototype moderate area near surface detection technologies
- Performed studies to deepen understanding of capillary trapping mechanism
- Hosted other academic institutions, gov. agencies and private sector entities in field experiment

Summary

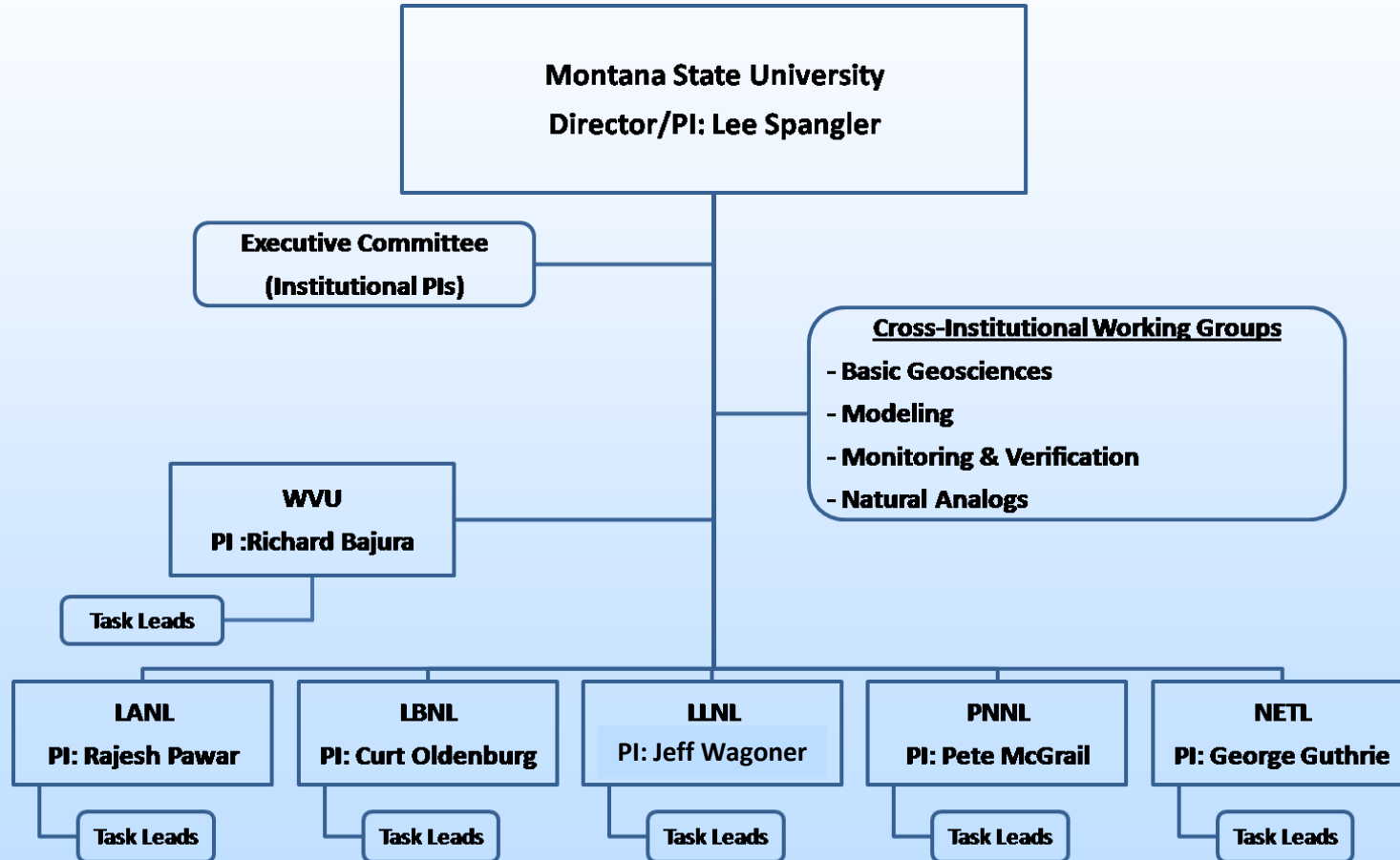
- Multiple computational codes have been improved
- Near surface detection technologies have been tested
- Analogs are providing important information to understanding of risk

Appendix

- These slides will not be discussed during the presentation, **but are mandatory**

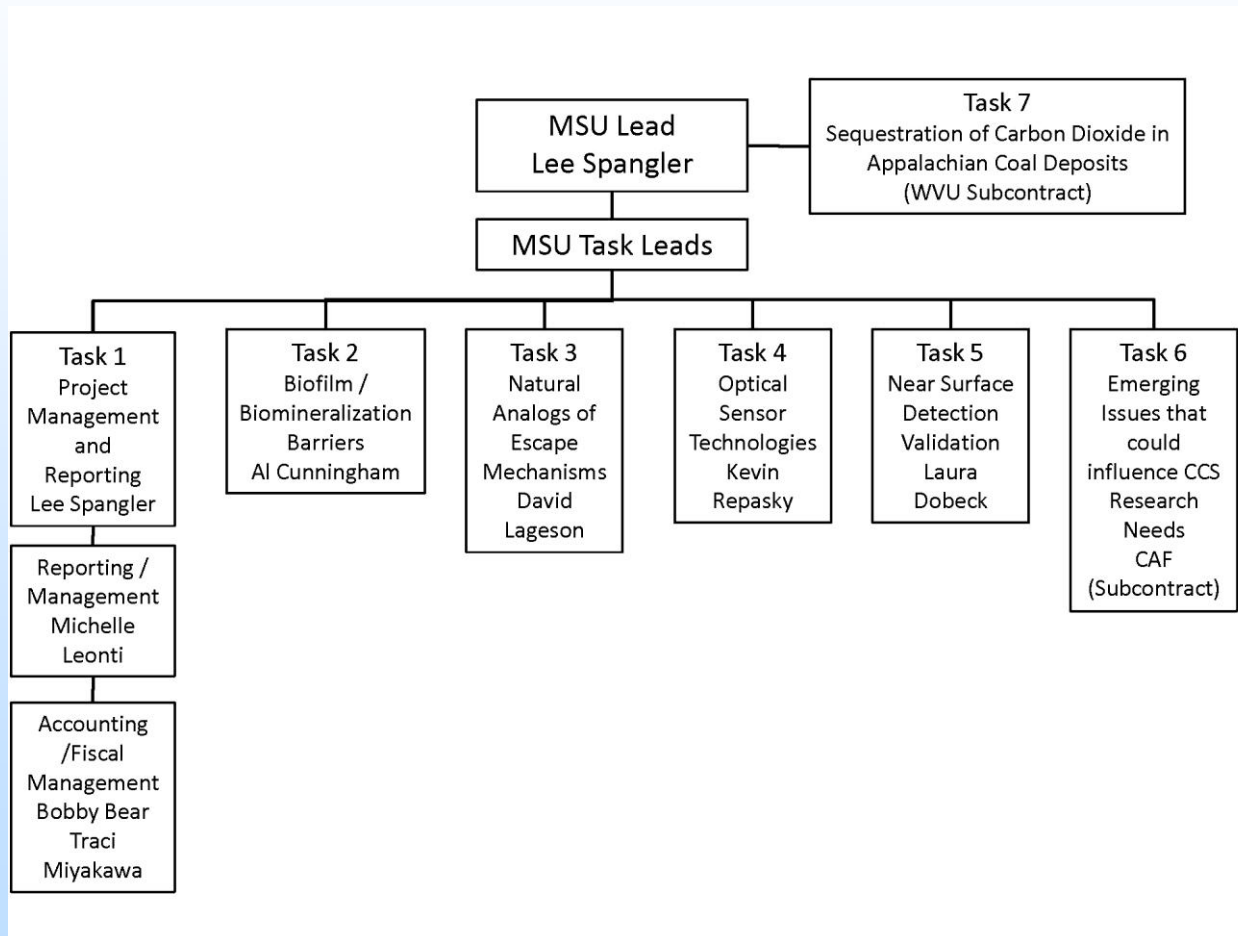
Organization Chart

Multi-Institutional Management Structure



Organization Chart

MSU Internal Management Structure



Gantt Chart

Task	Description (*)=see table below	Project Quarter									
		Q1	Q2	Q3	Q4	Q5	Q6	Q7	Q8	Q9	Q10
1	Project Management, Planning & Reporting	←————→									←
1.1	*	←————→									←
1.2	*	←————→									←
1.3	*	←————→									←
2	Biofilms and Biomineralization	←————→									←
2.1	*	←————→									←
2.2	*	←————→									←
2.3	*	←————→									←
2.4	*	←————→									←
2.5	*	←————→									←
2.6	*	←————→									←
2.7	*	←————→									←
3	Natural Analogs of Escap Mechanisms	←————→									←
3.1	*	←————→									←
3.2	*	←————→									←
4	Optical Detection for Carbon Sequestration	←————→									←
4.1	*	←————→									←
4.2	*	←————→									←
5	Validation near surface CO2 detection	←————→									←
5.1	*	←————→									←
5.2	*	←————→									←
5.3	*	←————→									←
5.4	*	←————→									←
5.5	*	←————→									←
5.6	*	←————→									←
6	Subcontract Crown Agro Fuels	←————→									←
6.1	*	←————→									←
6.2	*	←————→									←
7	Subcontract WVU	(Detail schedule will be provided later)									

The tasks are continued in the no-cost extension awarded in August 2012. The schedule will be finalized in the revised PMP to be submitted to DOE by November 2012.

Gantt Chart

Cont.

Task 1.0 – Project Management, Planning, and Reporting													
Subtask 1.1 Project Management													
Subtask 1.2 Project Reporting													
Subtask 1.3 Presentations and Briefings													
Task 2.0 – Biofilms and Biomineralization													
Subtask 2.1 Conduct experiments on CO ₂ biomineralization deposits on flat coupons and in porous media bead packs.													
Subtask 2.2 Develop method to control deposition rate of biomineralized calcium carbonate with distance along a porous media flow path.													
Subtask 2.3 Optimize biomineralization of isotopically labeled CO ₂ carbon under variable head space pressure.													
Subtask 2.4 Evaluate the potential for coalbed mediated CO ₂ sequestration.													
Subtask 2.5 Construct a system capable of flowing supercritical fluids through the bore of the magnet of the NMR spectrometer.													
Subtask 2.6 Evaluate transport phenomena for brine and supercritical CO ₂ using magnetic resonance techniques.													
Subtask 2.7 Evaluate transport phenomena for brine and supercritical CO ₂ in a bead pack or other model porous media.													
Task 3.0 – Natural Analogs of Escape Mechanisms													
Subtask 3.1 Leakage versus Confinement Associated with Subsurface Migration of Natural CO ₂ across Faults and Fracture Networks													
Subtask 3.2 Ancient Hydrothermal Plumes as a Natural Analog of Hydrofracting Caprocks and Geochemical Healing Mechanisms													
Task 4.0 – Optical Detection for Carbon Sequestration Site Monitoring													
Subtask 4.1 Underground Fiber Optic Sensors													
Subtask 4.2 UltraCompact Thermal Infrared Imagers													
Task 5.0 – Validation of Nearsurface CO₂ Detection Techniques and Transport Models at Experimental Field Site.													
Subtask 5.1 Seasonal Site Preparation													
Subtask 5.2 Coordinate experimental season with ZERT team.													
Subtask 5.3 Collect data in support of ZERT research project goals.													
Subtask 5.4 Investigate opportunities for greater involvement outside of the ZERT team.													
Subtask 5.5 Support optical remote sensing group													
Subtask 5.6 Support pollen capture of tracers experiments:													
Task 6.0 – Tracking Emerging Issues That Could Influence CCS Research Needs													
Subtask 6.1 Provide information to government at the state, federal and international levels.													
Subtask 6.2 Provide information to NGOs, industry groups, and professional groups relevant to CCS.													
Task 7.0 – Sequestration of Carbon Dioxide in Appalachian Coal Deposits (WVU Subcontract)													
(Detailed Task and Subtask descriptions will be provided at a later date.)													

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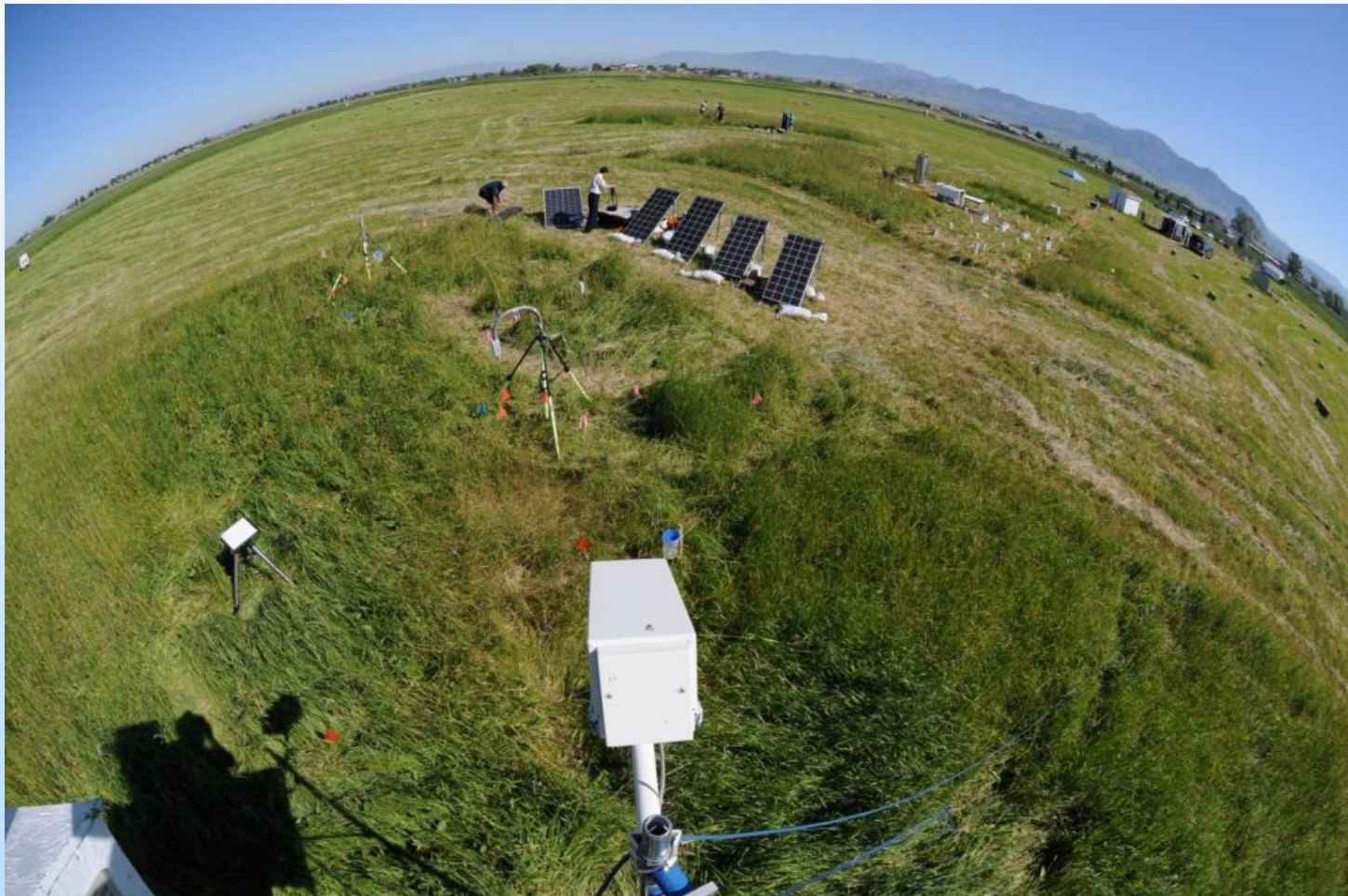
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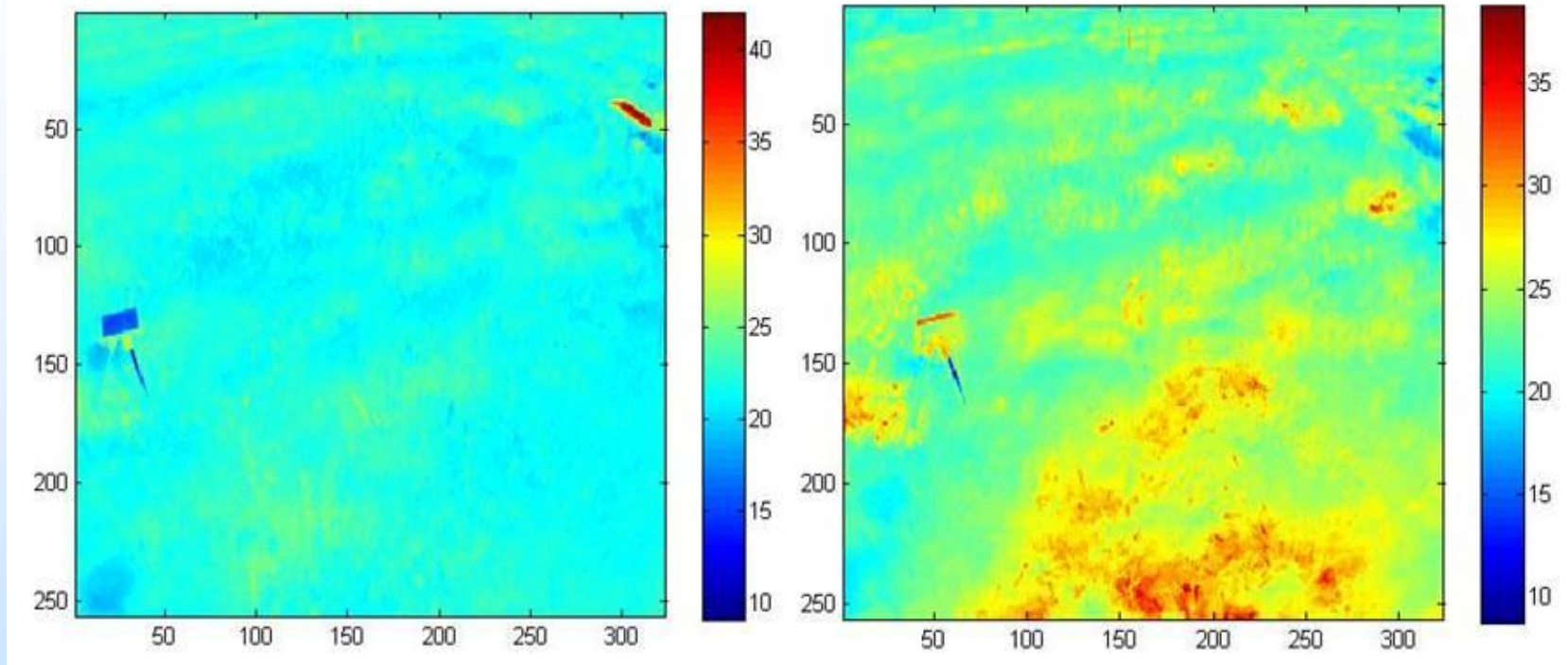
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Joseph Shaw

ZERT II Summary - August 3, 2012

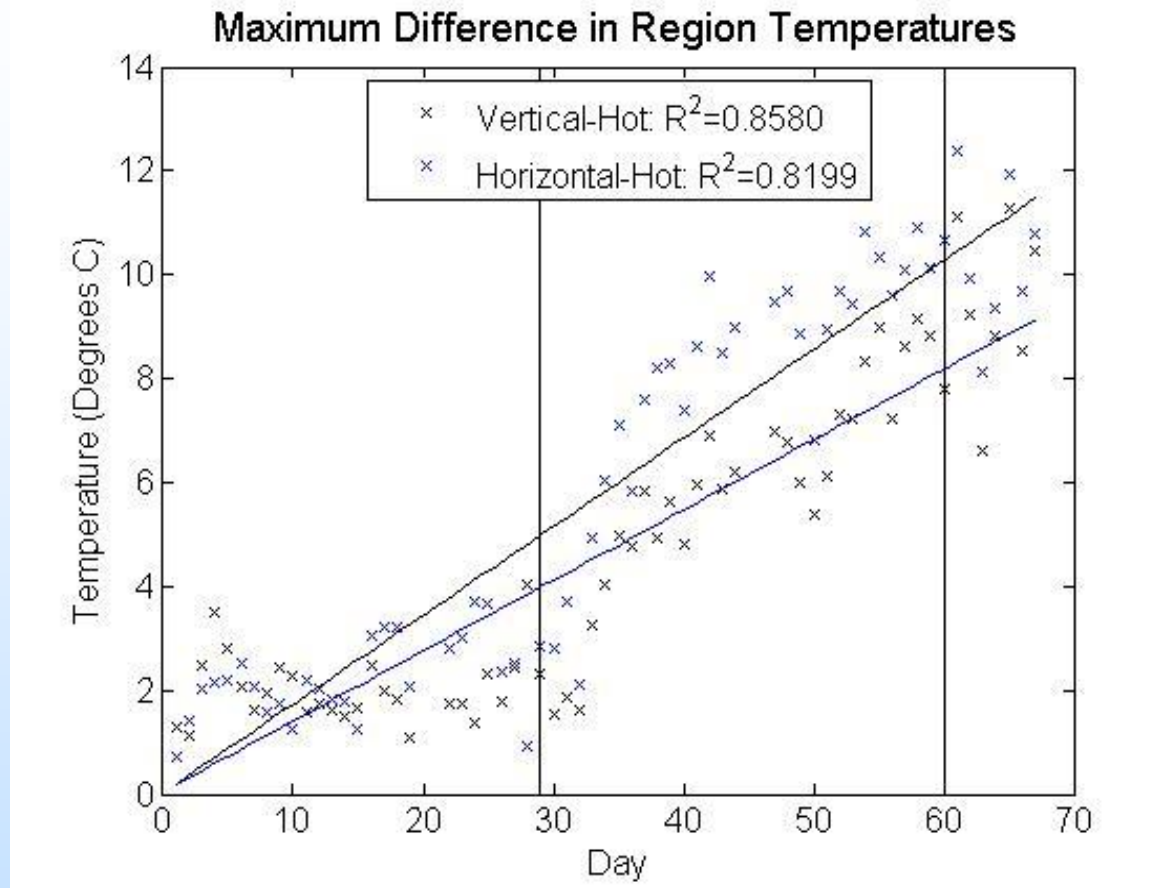


Long-wave thermal vegetation imaging to detect CO₂



Thermal images (°C) for 10 AM, 7/13/2011 (left) and 10 AM, 8/10/2011 (right). The right-hand image shows that the plant temperatures are much higher with high CO₂ flux (the -1,0) hot spot is just outside the lower-right corner).

Long-wave thermal vegetation imaging to detect CO₂



2011 ZERT release data from thermal camera, showing hotspot-control temperature difference. As the vegetation becomes more stressed near the hotspot, it loses ability to self-regulate its temperature. The result is a higher vegetation temperature that can be seen almost immediately after the start of the release (left-hand vertical black line). During the previous month, the difference was very stable.

Remote weather sensors

Undergraduate & graduate students working on solar-powered wireless network for remote weather station.

New electrical grounding helped us survive a Lightning strike in July 2012 that shut down The rest of the ZERT site.

