SAND2014-3289C

INTERCALATION OF CO_2-H_2O BY CLAY MINERALS

Research Team

Randall T. Cygan, Evgeniy Myshakin, Wissam A. Saidi, Vyacheslav N. Romanov, and Kenneth D. Jordan (Sandia, NETL, and U of Pittsburgh)

Objectives of Research

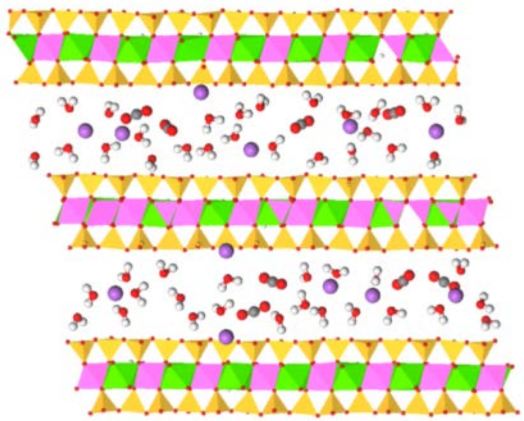
Develop accurate molecular models of CO_2-H_2O structure and dynamics in interlayer of Na-montmorillonite, and confirm experimental carbon capture by clay

Conclusions

Classical and DFT models show degree of swelling caused by intercalation of CO_2 strongly depends on the initial H_2O content in the interlayer space and that CO_2 intercalation stimulates inner-sphere adsorption of interlayer Na^+ on the internal clay surfaces, which modifies the wetting properties of the surfaces

Impact on Geological Carbon Storage

Identified molecular basis for CO_2 capture by smectite clays and their swelling behavior, which will influence permeability, mechanical strength, and integrity of shale-mudstone caprock



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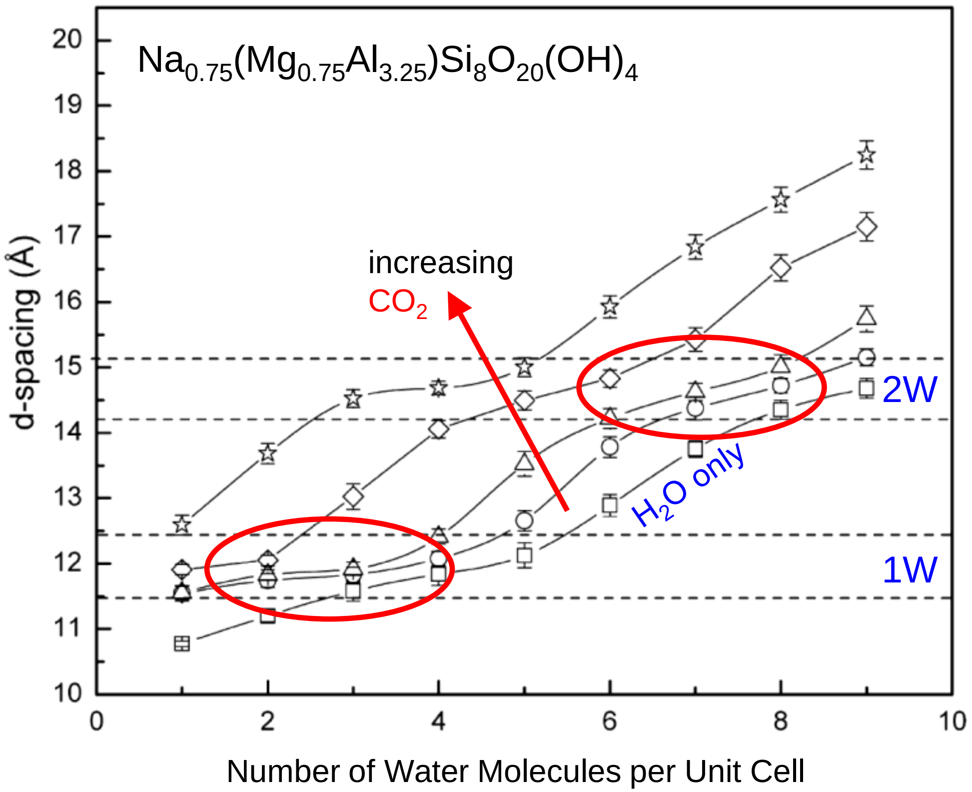
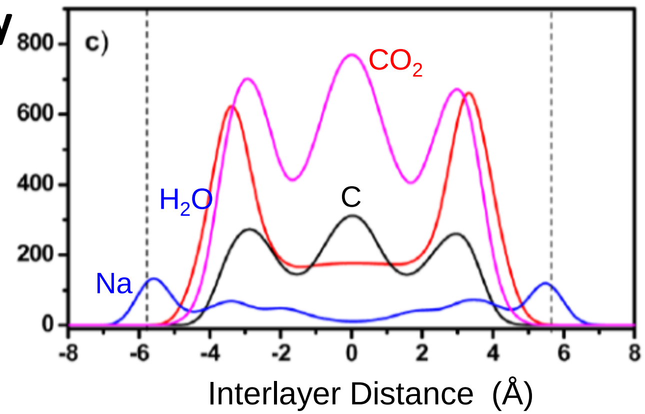
INTERCALATION OF CO_2-H_2O BY CLAY MINERALS

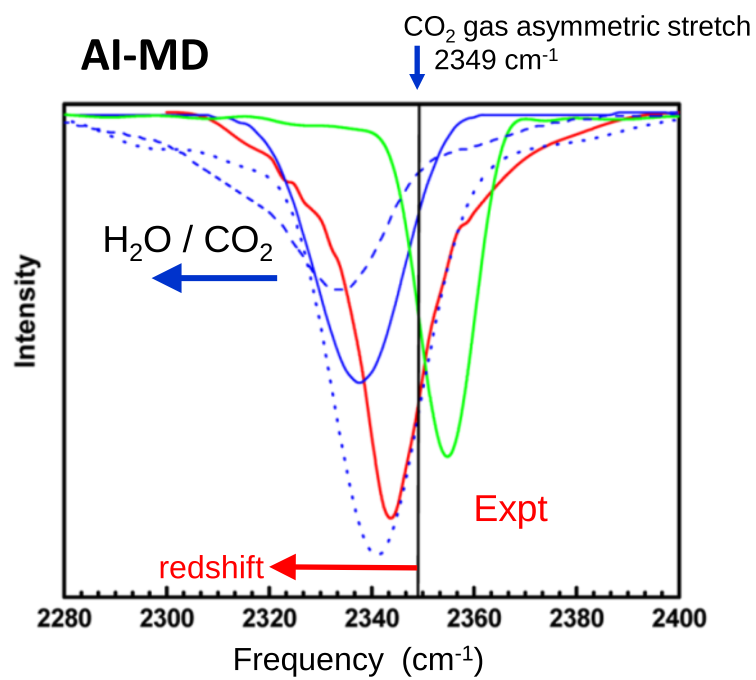
MD 348 K and 13 MPa



Density Profile



AI-MD



EULERIAN-LAGRANGIAN NUMERICAL METHODS FOR TRANSPORT SIMULATIONS

Research Team

Todd Arbogast, Jamie Pool (UT-Austin), Chieh-Sen Huang (Nat'l Sun Yat-sen Univ., Taiwan)

Objectives of Research

Numerically simulate transport processes over very long time periods

Requirements

Preserving physics:

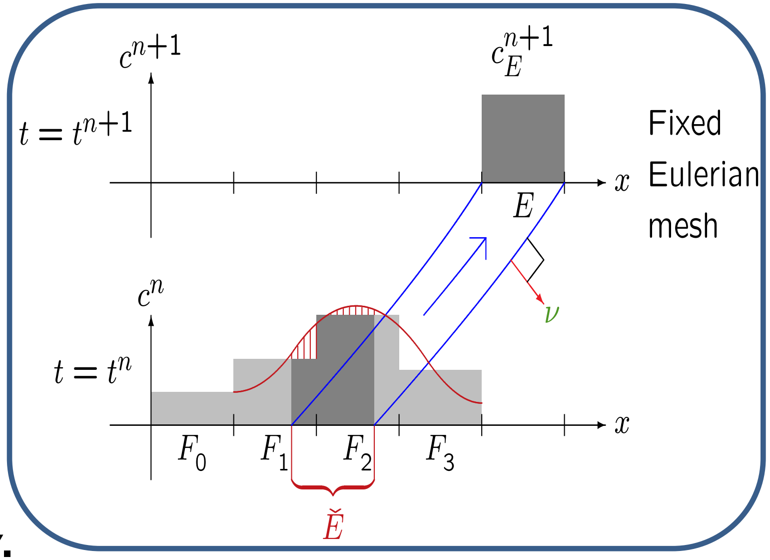
- Mass is conserved locally over the computational mesh.
- The concentration has no or minimal over- and under-shoots.
- Mass experiences minimal numerical diffusion.

Numerical efficiency:

- Accuracy on coarse meshes (reservoirs are large).
- Explicit computations (efficient in parallel vs. implicit).
- High order accuracy (more efficient in parallel).
- No CFL time step constraint (time stepping is serial).

  Fixed-mesh methods have a CFL restriction

  $\Delta t \leq h/\max|u(x)|$, h=mesh spacing



Approach

Eulerian-Lagrangian methods have the desired properties, *if they can be implemented appropriately*.

EULERIAN-LAGRANGIAN NUMERICAL METHODS FOR TRANSPORT SIMULATIONS

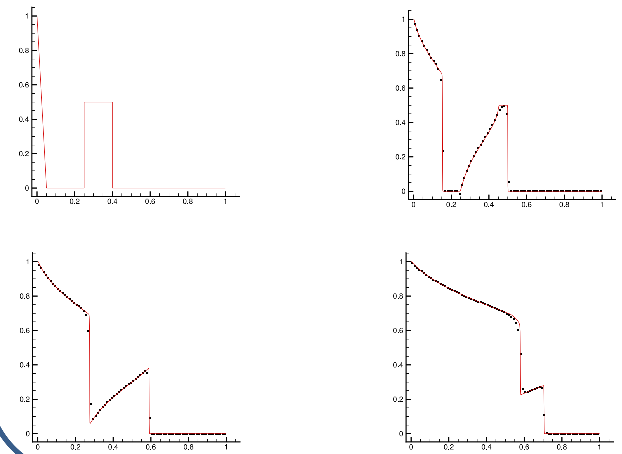
Conclusions **Numerical results show:**

- Use of long time steps and coarse grids
- Relatively low numerical diffusion
- Essentially non-oscillatory
- Formal $O(h^5)$ realized for smooth solutions
- Mass conservation

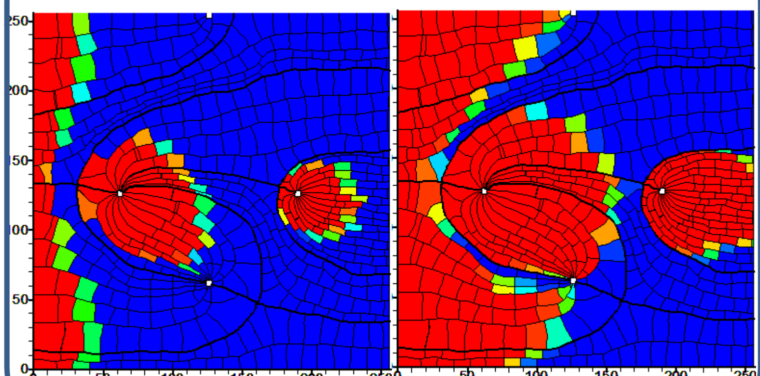
Impact on Geological Carbon Storage

Potential for efficient use of massively parallel computers for long-time CO_2 simulations.

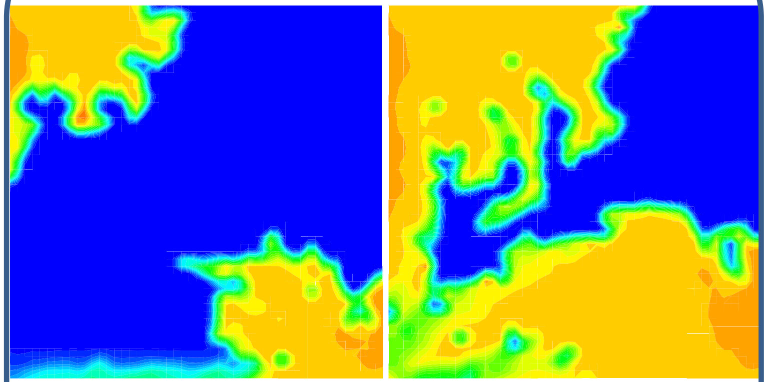
A Buckley-Leverett Problem



Stream-tube Mesh



Two-Phase Flow



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A global Jacobian method for mortar discretizations of a fully-implicit two-phase flow model

Research Team

– Ben Ganis, K. Kumar, G. Pencheva, M.F. Wheeler, I. Yotov

Objectives of Research

– Develop fast numerical algorithms for multiscale mortar methods with fully-implicit two-phase flow including capillarity, compressibility, and gravity in 3D.

Conclusions

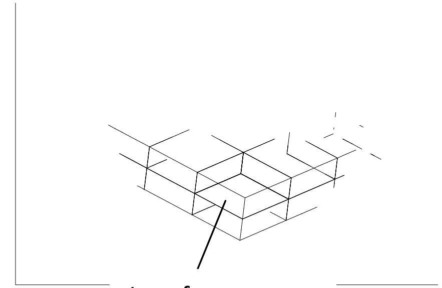
– Showed significant speedup in run time by performing fewer Newton iterations.

– Improved saturation accuracy through accurate phase mobility upwinding.

Impact on Geological Carbon Storage

– Allows stuctured grid codes to easily consider non-matching grid geometry.

– Enables use of linear preconditioners with nonlinear models for faster results.

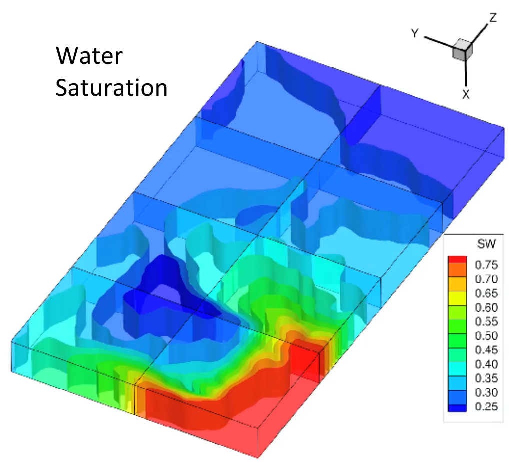


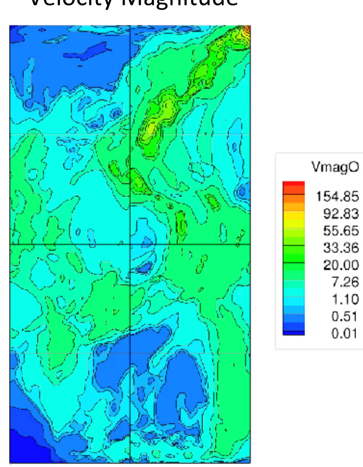
Global Jacobian System:

$$\begin{bmatrix} J_{\Theta\Theta} & J_{\Theta\Lambda} \\ J_{\Lambda\Theta} & J_{\Lambda\Lambda} \end{bmatrix} \begin{bmatrix} \delta\Theta \\ \delta\Lambda \end{bmatrix} = \begin{bmatrix} R_\Theta \\ R_\Lambda \end{bmatrix}$$

$$\delta\Theta = \begin{bmatrix} \delta P_o \\ \delta N_o \end{bmatrix}, \quad \delta\Lambda = \begin{bmatrix} \delta\Lambda_1 \\ \delta\Lambda_2 \end{bmatrix}$$

Heterogeneous Example with 8 subdomains:





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Simulating Fluid-Induced Discrete-Fracture Propagation using Random Finite-Element Meshes

Research Team

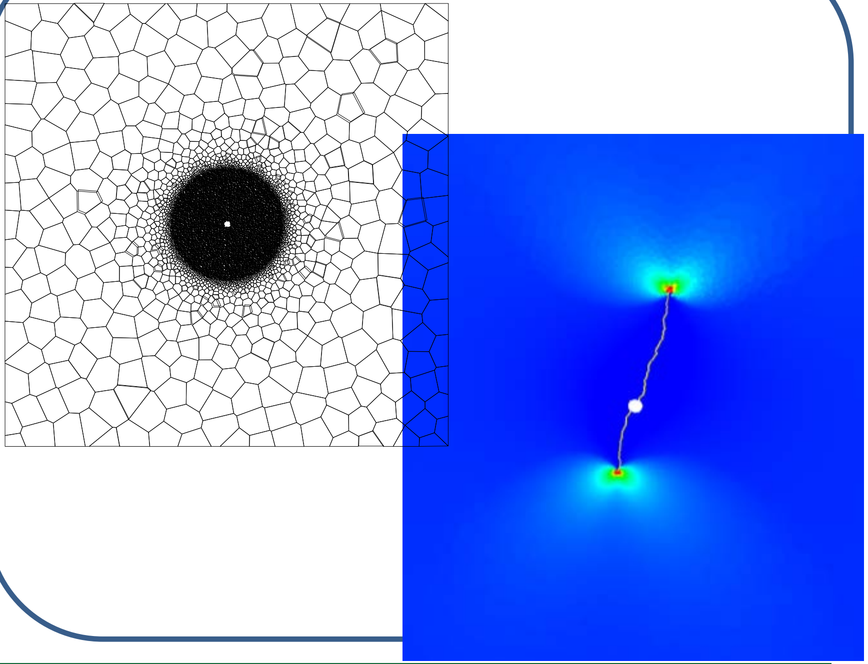
Joe Bishop and Martinez, M.

Objectives of Research

- Demonstrate the viability of using random close-packed Voronoi meshes to model fluid-induced fracture propagation.
- Demonstrate mesh convergence in a distributional (probabilistic) sense.
- Demonstrate that random meshes are consistent with material heterogeneity.

Conclusions

The use of random meshes is a viable numerical approach for modeling fluid-induced fracture propagation.



Impact on Geological Carbon Storage

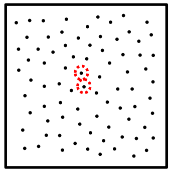
- This numerical method can be used to assess the caprock integrity by predicting the reactivation and propagation of existing fractures or the nucleation of new fractures.
- Can be used to model subcritical fracture growth by developing an appropriate multiphysics cohesive-zone model.

Simulating Fluid-Induced Discrete-Fracture Propagation using Random Finite-Element Meshes

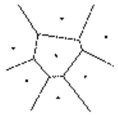
Fracture Modeling

- Each Voronoi cell is formulated as a finite element
- Cohesive-zone models are used to model energy dissipation at the crack tip.
- Connectivity of mesh is modified to allow fracture to propagate.

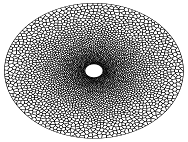
Random Voronoi Meshing



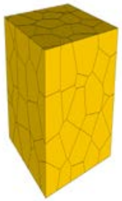
Maximal Poisson Sampling of a domain



Voronoi Structure

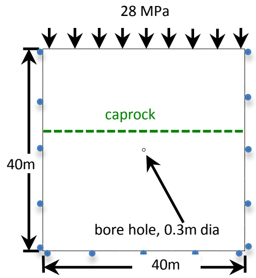


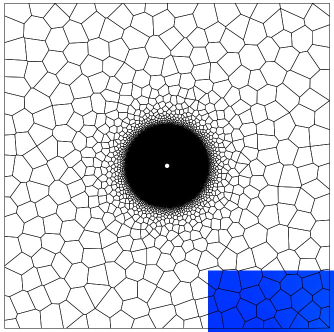
Example Voronoi mesh in 2D



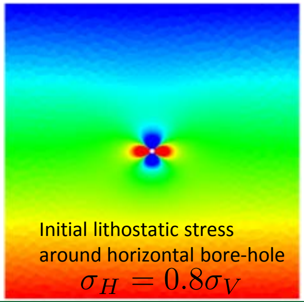
Example Voronoi mesh in 3D

Hydraulic Fracturing Example

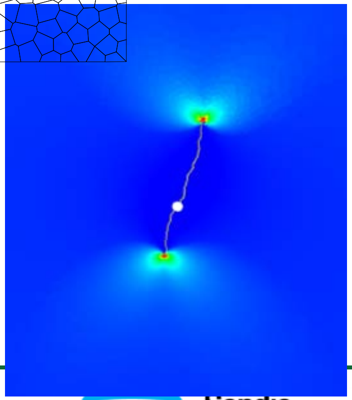




Graded Voronoi mesh around bore-hole



Initial lithostatic stress around horizontal bore-hole $\sigma_H = 0.8\sigma_V$



Resulting fracture propagation

Cohesive Element Model for Fracture Propagation in Limestone

Research Team

Alex Rinehart and Joseph Bishop

Objectives of Research

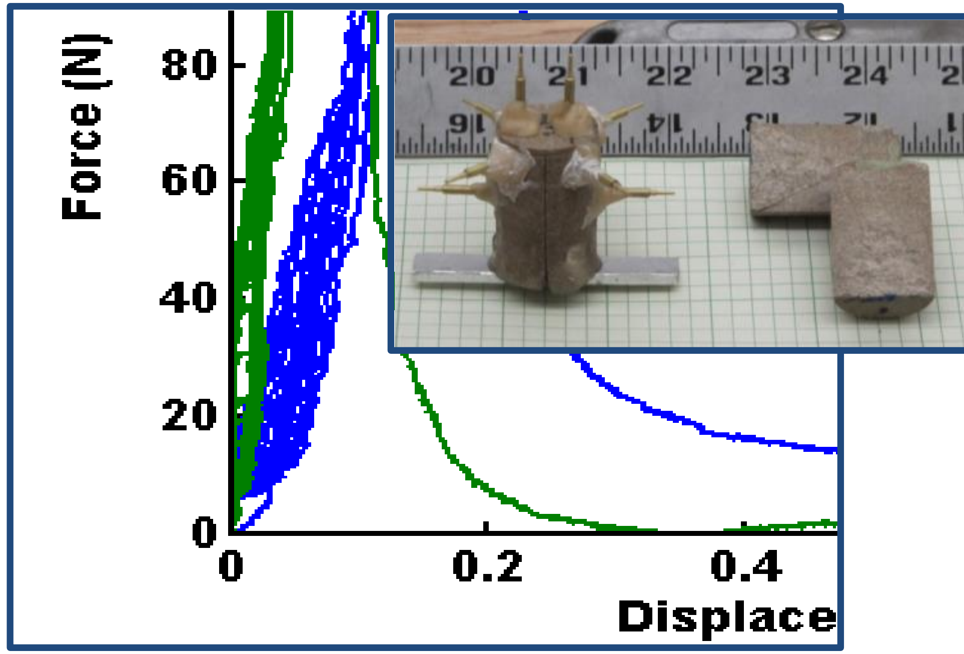
Develop and test cohesive model for crack propagation in geomaterials.

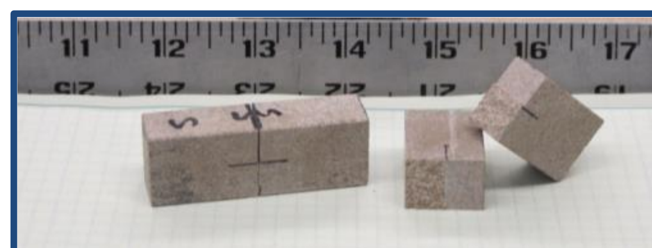
2 geometries of fracture toughness measurements.

Develop finite/cohesive models in Abaqus.

'Match' short-rod test results with model.

Test that cohesive element model is geometry independent with second test-type.





Cohesive Element Model for Fracture Propagation in Limestone

Conclusions

Performed experiments.

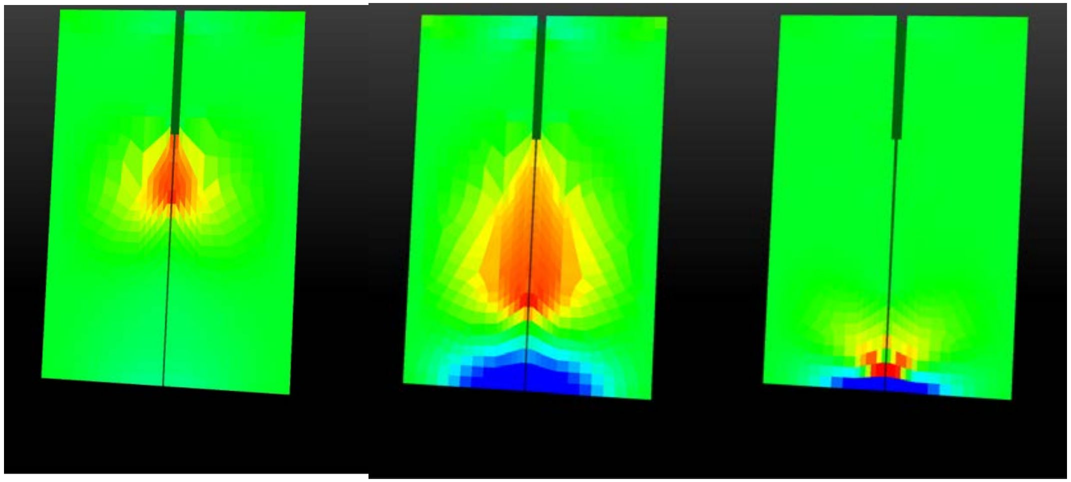
Running Abaqus model for short-rod geometry with characteristic limestone properties.

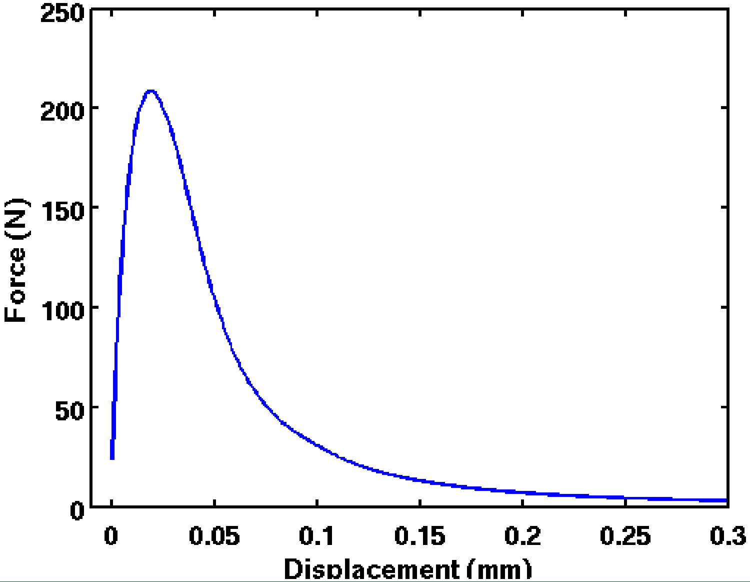
Beginning calibration and 3pb development.

Impact on GCS

Links experimental fracture measurements to subsurface modeling.

Foundation for modeling sub-critical cracking and chemical effects on fracture.





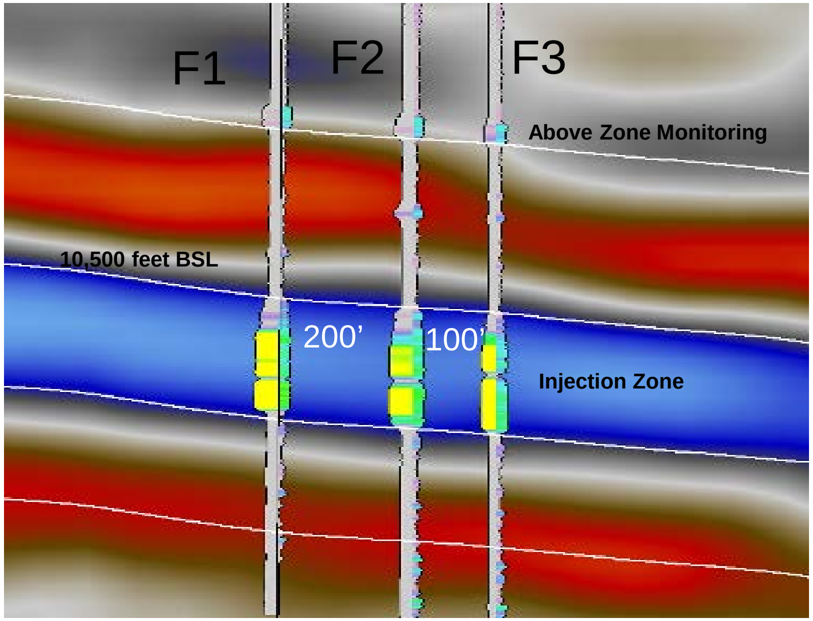
Detection of well-bore geomechanical effects in Cranfield reservoir with ensemble-based algorithms

Research Team

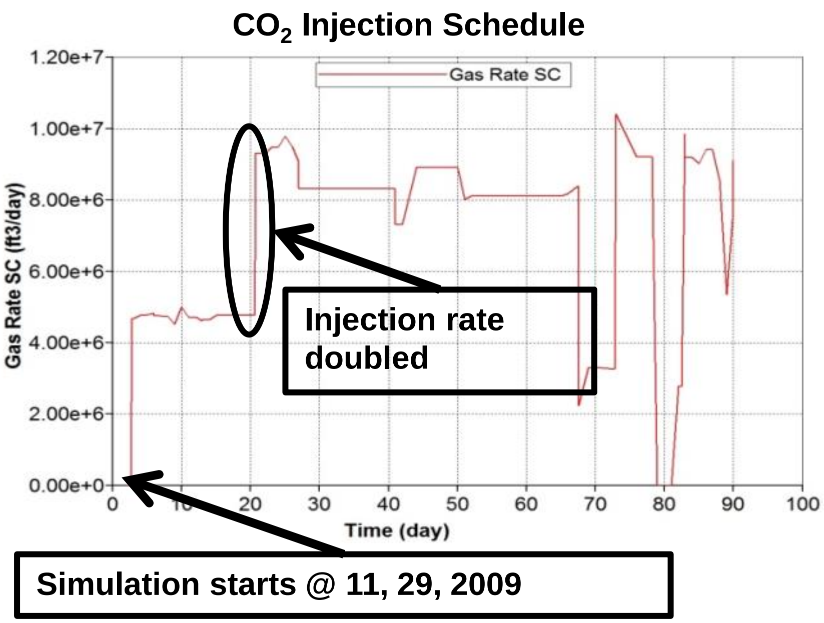
Reza Tavakoli, Mary F. Wheeler, Mojdeh Delshad

Objectives of Research

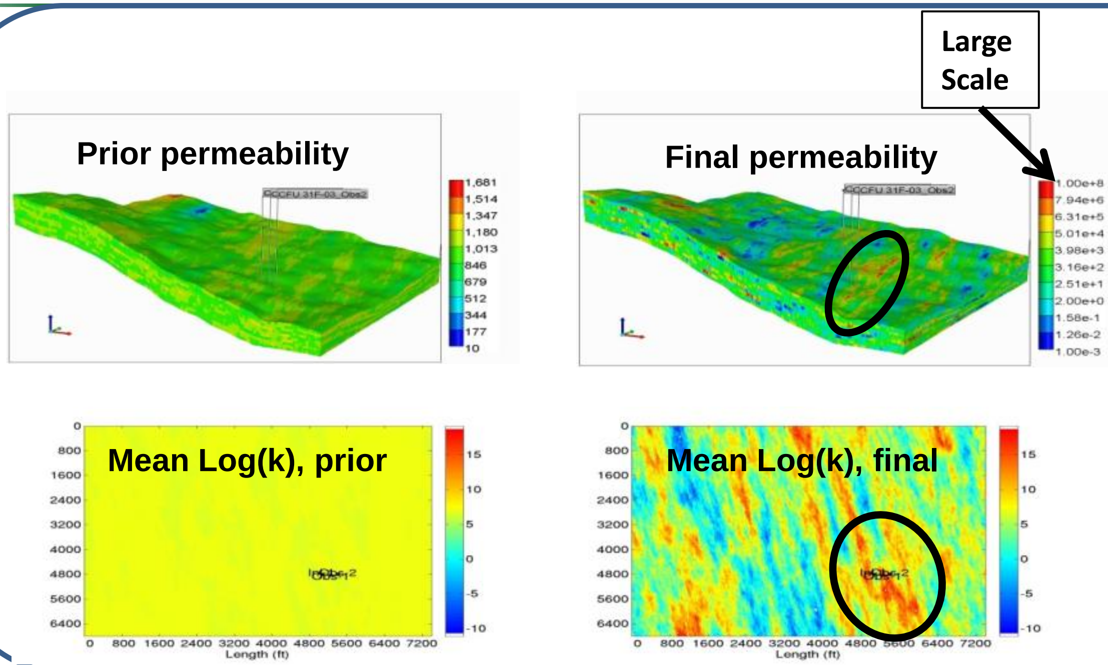
Develop algorithmic approaches to integrate the dynamic (flow and geomechanical) observation into reservoir models in order to correctly inform models for reliable predictions



CO_2 Injection Well: F1
Monitoring Wells: F2, F3



Detection of well-bore geomechanical effects in Cranfield reservoir with ensemble-based algorithms



After integration of injection data (BHP, CO_2 breakthrough), the prior moderate values of permeabilities (top-left) around injection well increased dramatically to very large values (top-right). These results confirm the possibility of occurrence of geomechanical effects (fracturing) as a consequence of doubling the CO_2 injection rate.

Conclusions

It is essential to couple multiphase flow and geo-mechanics simulations associated with parameter estimation to accurately understand the subsurface processes and to predict a consequence of geological storage of CO_2.

Impact on Geological Carbon Storage

The ensemble-based algorithms will offer effective CO_2 monitoring that not only predict the fate of CO_2 underground but also estimate the uncertainty in the prediction.

Joint inversion for coupled quasi-static poroelasticity

Research Team

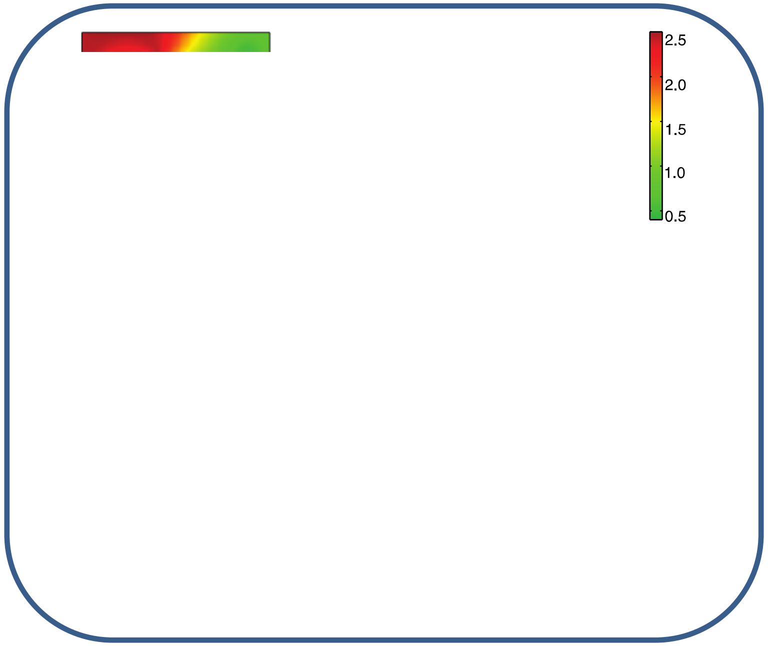
Marc A. Hesse and Georg Stadler

Objectives of Research

InSAR based monitoring of pressure plume and reservoir characterization

Conclusions

Surface uplift gives a good image of the subsurface pressure distribution (horiz. aquifer).
Identification high-permeability pathways require high-frequency data.
Flow barriers can be identified with confidence.



Impact on Geological Carbon Storage

Satellite geodesy provides a relatively low cost method of monitoring the pressure plume created by geological CO_2 storage.

Incorporation of time-series surface deformation improves the characterization of large-scale horizontal permeability variations.

May help to avoid pressure build up on critically stressed pre-existing faults.

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Inversion methodology

Joint inversion

- surface displacements
- hydraulic heads

Bayesian inference of permeability

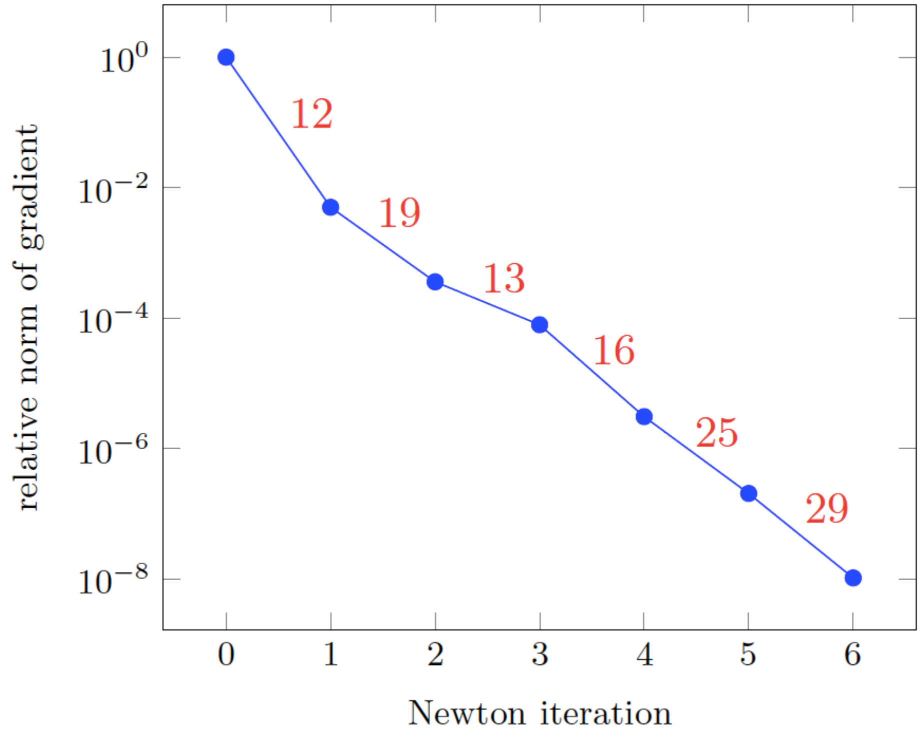
- Computation of MAP
- Gaussian approximation of posterior

Efficient optimization

- Gradient computation using adjoints
- Gauss-Newton method

Future work

- Simultaneous inference of mechanical and hydraulic parameters
- Application to field site (need data)



A Consideration of Foam for CO_2 Storage

Xianhui Kong

Mojdeh Delshad, Mary Wheeler

Center for Subsurface Modeling

The University of Texas at Austin

4/3/2014

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A Consideration of Foam for CO_2 Storage

Research Team

– Center for Subsurface Modeling

Objectives of Research

– Review foam application in CO_2 sequestration
– Develop flow model for surfactant-stabilized CO_2 foam in deep saline aquifers
– Optimize CO_2 injection for maximum storage

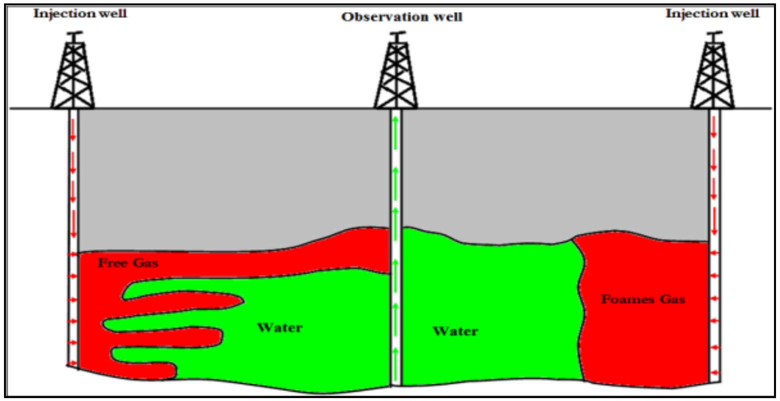
Conclusions

– Foam can be generated by injection of water soluble surfactant and CO_2 at high pressure/temperature
– Foam significantly reduces CO_2 mobility and slow down its upward migration

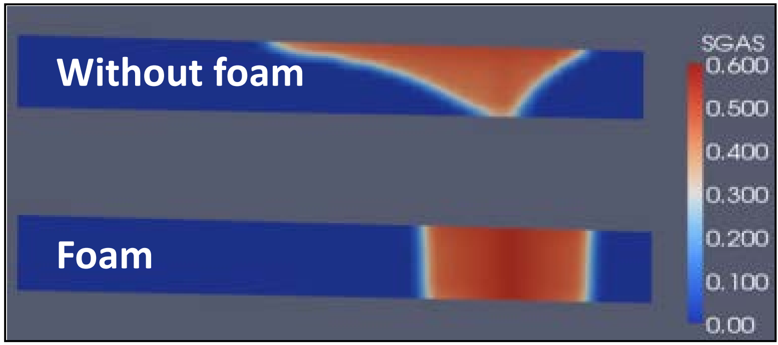
Impact on Geological Carbon Storage

– Mobility control and conformance control
– Reduces mobility ratio with CO_2 foam and improves CO_2 displacing and sweep efficiency
– Mitigates leakage through high permeability zone
– Improved dissolution and residual trapping

Foam for conformance control



CO_2 saturation with/o foam (IPARS)



Bridging from Pore to Continuum: A Hybrid Mortar Domain Decomposition Framework for Subsurface Flow and Transport

Research Team

Yashar Mehmani and **Matthew Balhoff**

Objectives of Research

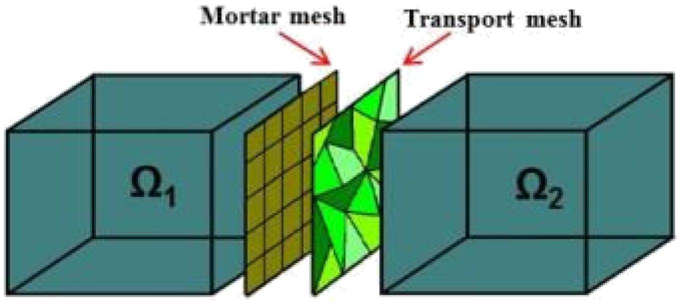
Develop a hybrid mortar domain decomposition framework for parallel modeling (linear and nonlinear) flow and transport across scales and in large pore-scale domains.

Conclusions

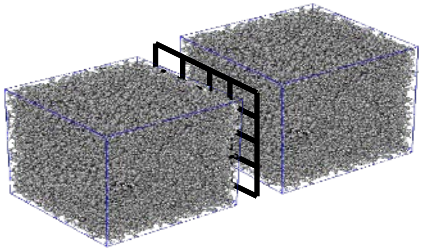
- Efficient mortar methods were developed for coupling flow and transport
- Methods were shown to be much more efficient than solving the domain as a whole

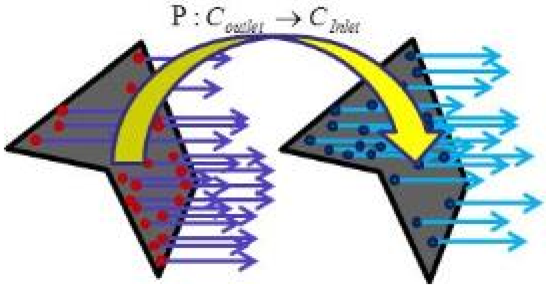
Impact on Geological Carbon Storage

New algorithms can be used to predict advective/diffusive/reactive transport across scales.

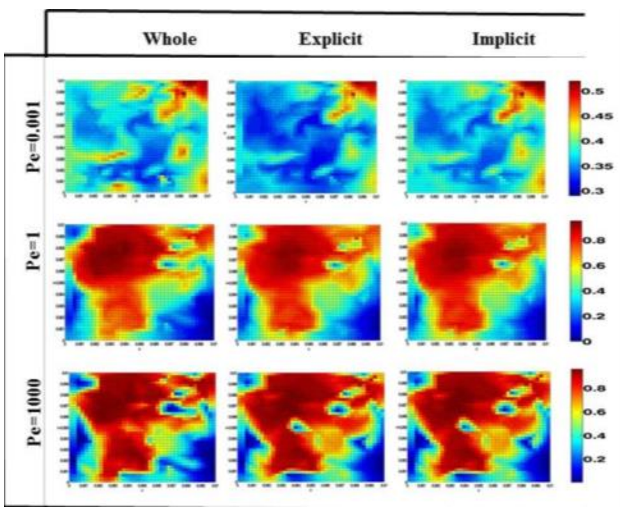


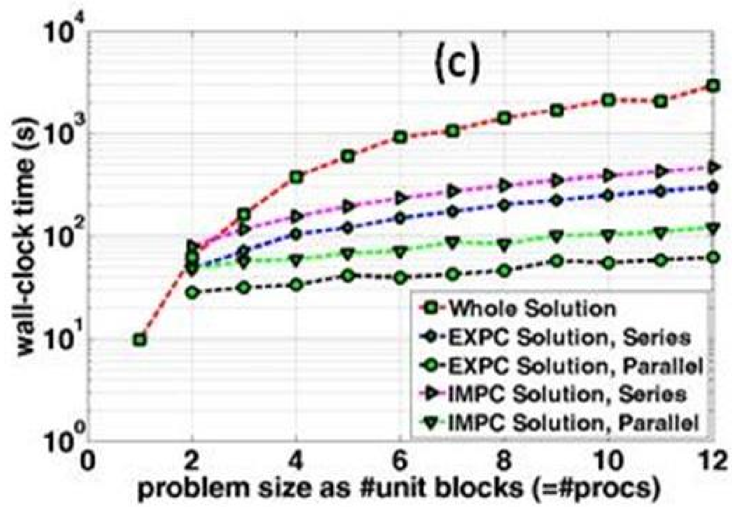
Bridging from Pore to Continuum: A Hybrid Mortar Domain Decomposition Framework for Subsurface Flow and Transport





- Developed a "global mortar formulation" for flow and transport
- EXPC and IMPC scheme for coupling transport; EXPC faster and easier
- Concentration and pressure fields at interface match full solution well
- Domain decomposition much FASTER than solving full solution, even in series





A Streamline Splitting Pore-Network Approach for Computationally Inexpensive and Accurate Simulation of Species Transport in Porous Media

Research Team

Yashar Mehmani and Matthew Balhoff

Objectives of Research

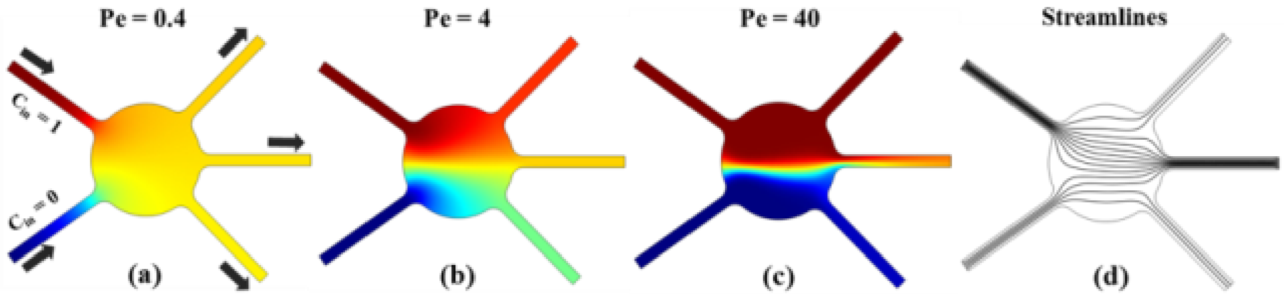
Develop a accurate and efficient model for predicting transverse dispersion in porous media, based on an accurate description of pore-scale mixing

Conclusions

- Model compares very well against micromodel experiments and direct numerical methods
- Model is very efficient and can predict transverse dispersion coefficients for macro-models

Impact on Geological Carbon Storage

Accurate transverse dispersion coefficients can be extracted in a short period of time to be used in macro-scale models of CO_2 transport



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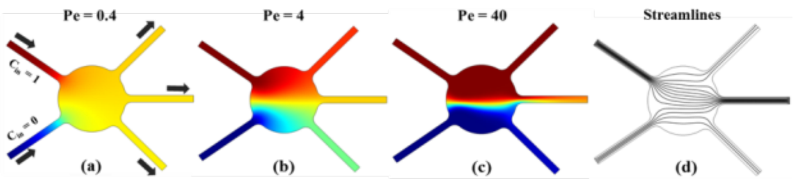
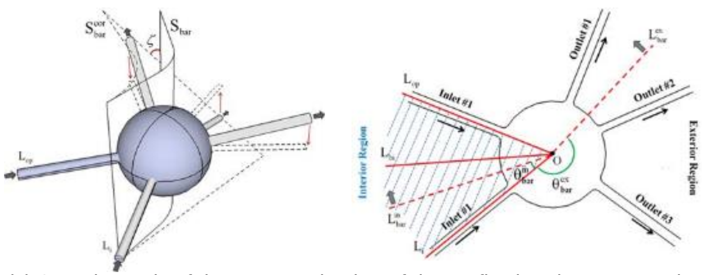
A Streamline Splitting Pore-Network Approach for Computationally Inexpensive and Accurate Simulation of Species Transport in Porous Media

Motivation



Schematic of steady state concentration fields for a typical pore at different Pe and streamline field obtained from flow equation.

Streamline Splitting Approach



(a) 3D schematic of the pore, projection of the outflowing throats onto the *flowing plane*, the *barrier surface*, and the *transverse angle* corresponding to the twisting of the *barrier surface*. (b) 2D projection of all throats on the *flowing plane* (on P_{fl})

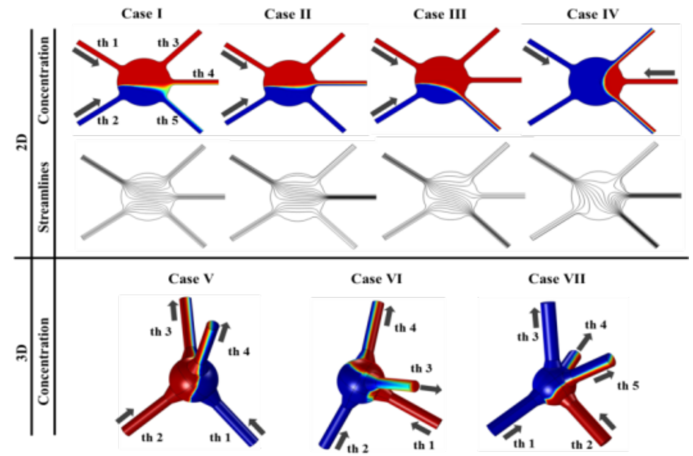
$$F_i(\vec{y}_{io}) := \sum_{i=1}^{N_i}\sum_{o=1}^{N_o}\omega_{io} y_{io}^2$$

$$\sum_{o=1}^{N_o}(-1)^{\beta_{io}} y_{io} |q_o| = C_i \qquad i = 1,\dots,N_i$$

$$\sum_{i=1}^{N_i}(-1)^{\beta_{io}} y_{io} = C_o \qquad o = 1,\dots,N_o$$

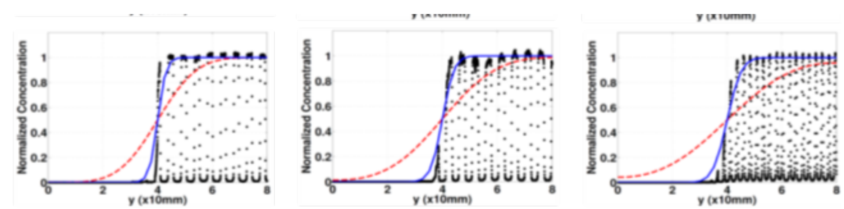
$$y_{io}(\in[0,1]) = \begin{cases} x_{io} & if \quad o \in Pr_i^c \\ 1 - x_{io} & if \quad o \in Pr_i \end{cases} \qquad \beta_{io} = \begin{cases} 1 & o \in Pr_i \\ 0 & o \in Pr_i^c \end{cases}$$

Verification with CFD models



Concentration fields of a dummy tracer (injected through one inlet) obtained from COMSOL simulations on one 2D pore and three distinct 3D pores.

Validation with Experiments



Concentration profiles along the 0.5, 1 and 1.5 cm transect lines including experimental data (dots), *SSM* transects (solid blue line), and *MCM* transects (dashed red line)

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Extended Roof snap-off for a continuous nonwetting fluid and an example case for supercritical CO_2

Research Team

Wen Deng, M. Bayani Cardenas, Philip C. Bennett

Objectives of Research

Develop a more comprehensive snap-off criterion as an extension to Roof snap-off criterion for continuous plumes

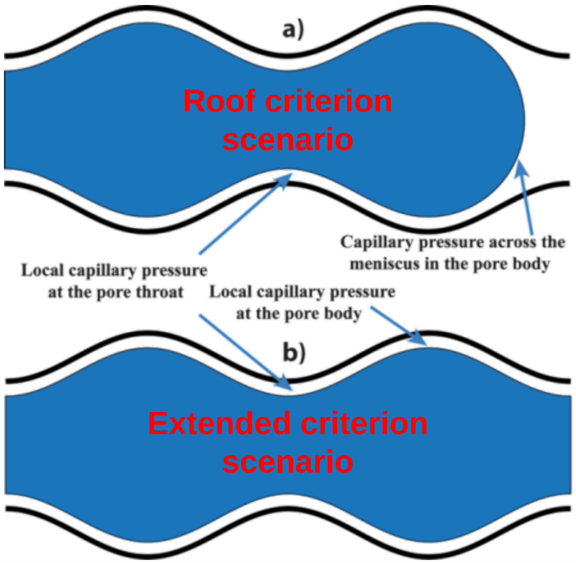
Conclusions

(1) The extended snap-off criterion works! It has been validated against CFD simulations

(2) Snap-off might be more frequent than predicted by the Roof snap-off criterion

Impact on Geological Carbon Storage

Residual trapping of CO_2 due to the snap-off during the imbibition process of CO_2 injection might occur more frequently than predicted by the classic snap-off criterion



Extended Snap-off Criterion

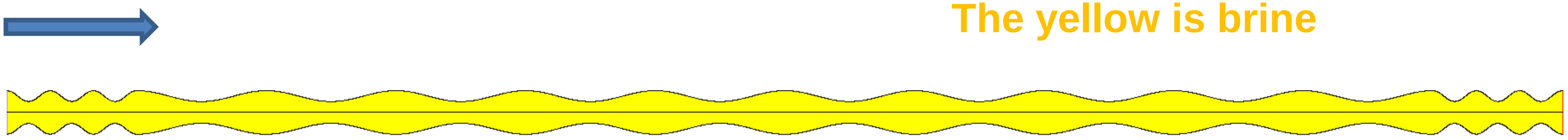
- **Snap-off and trapping of CO_2 droplets in the circular pore**

Example

Drainage

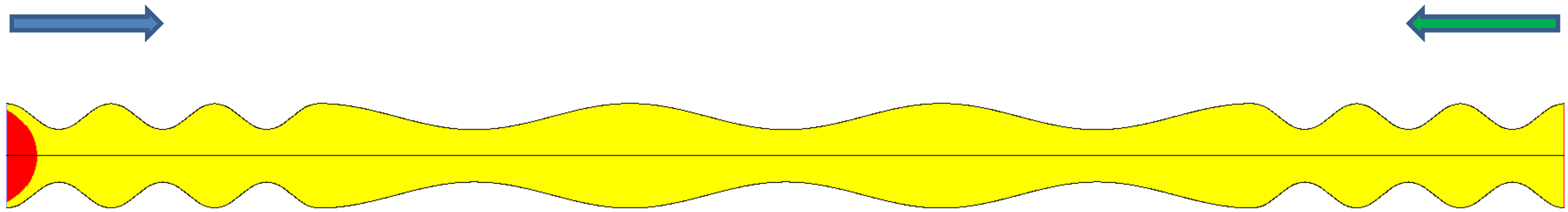
The red is supercritical CO_2

The yellow is brine



Drainage

Imbibition



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Pore scale reactive transport in microfluidic pore network system: calcium carbonate precipitation and dissolution

Research Team

Hongkyu Yoon and Tom Dewers

Objectives of Research

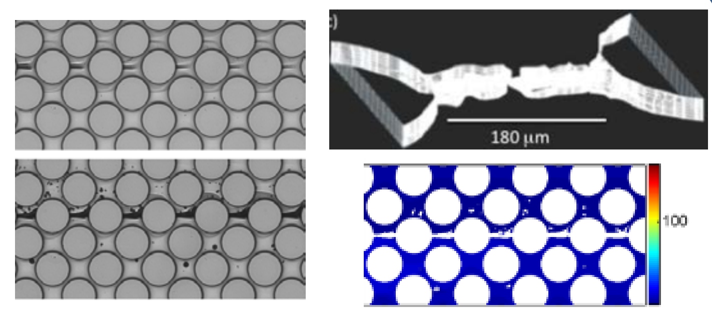
Determine calcium carbonate crystal morphology, precipitation rate, reactive surface area, and porosity relationships under flow and mixing conditions using laser scanning confocal microscopy and validate 3-D pore-scale reactive transport model

Conclusions

In-situ 3-D measurement of CaCO3 precipitation and dissolution will allow us to reveal fundamental mechanisms of CaCO3 crystal growth and porosity occlusion under flow conditions and develop quantitative relationships of reactive surface area, porosity, and permeability

Impact on Geological Carbon Storage

- Improve fundamental understanding of (1) crystal growth mechanism under flow conditions and (2) carbonate water-rock interactions at pore-scale
- Develop upscaled reaction rates at continuum scale



2-D optical Image of experimental $CaCO_3$ precipitates (left), 3-D confocal microscopy image of precipitates (upper right), and simulated $CaCO_3$ saturation ratio (lower right) at 8 hrs after start of experiment.

Contact angle measurements of supercritical CO_2-brine-rocks/minerals using X-ray computed tomography with intact samples

Research Team

Eric Guiltinan, Bayani Cardenas, Kuldeep Chaudhary, Jessie Maisano, Phil Bennett

Objectives of Research

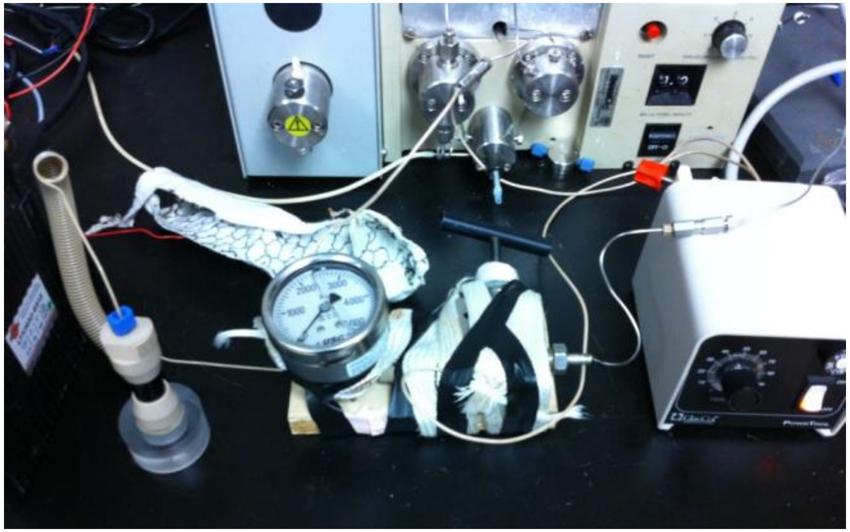
Characterize wettability alteration of s-CO_2/brine system using typical and intact reservoir/caprock materials

Conclusions

Work in Progress. Wettability alteration in capillary tubes can be effectively imaged at reservoir conditions using x-ray computed tomography.

Impact on Geological Carbon Storage

Previous work has focused on the wettability alteration of minerals such as mica, quartz, and glass. The wettability of reservoir rocks with respect to CO_2 is important because it impacts the amount of CO_2 sequestered due to capillary and structural trapping.



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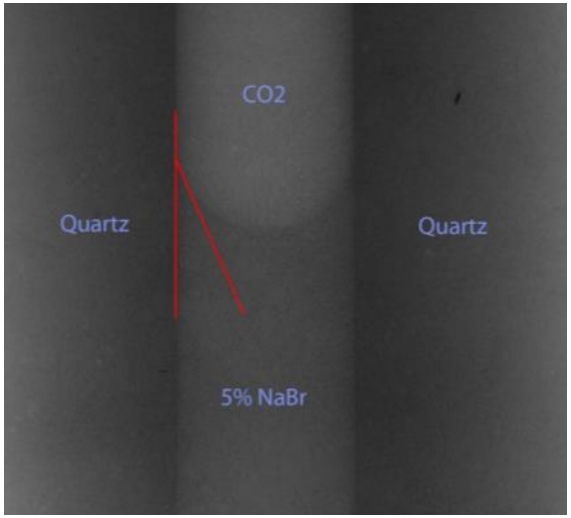
Contact angle measurements of supercritical CO_2-brine-rocks/minerals using X-ray computed tomography with intact samples

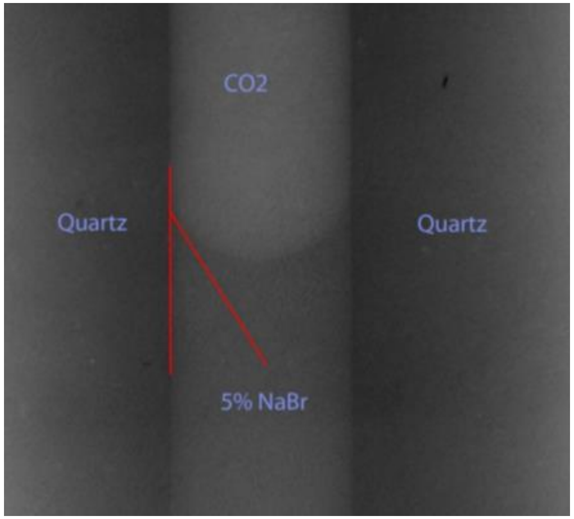
Progress

- Wettability alteration on quartz was recently imaged using XRCT
- The quartz images will be processed in Matlab and compared to previous results to validate the technique
- Shales, siltstones and other reservoir rocks will be analyzed
- Empirical equations of state will be developed to relate temperature, pressure, and brine concentration to wettability/contact angle.

6 mm diameter cores
1 mm diameter capillary



60 °C, 1400 psi (bar or Pa)



60 °C, 2600 psi (bar)

Experimental and molecular dynamics simulations of contact angle for carbon dioxide, brine, and muscovite systems

Research Team

Craig M. Tenney, Edward Matteo, Eric Guiltinan, Kuldeep Chaudhary, Randall T. Cygan, Bayani Cardenas

Objectives of Research

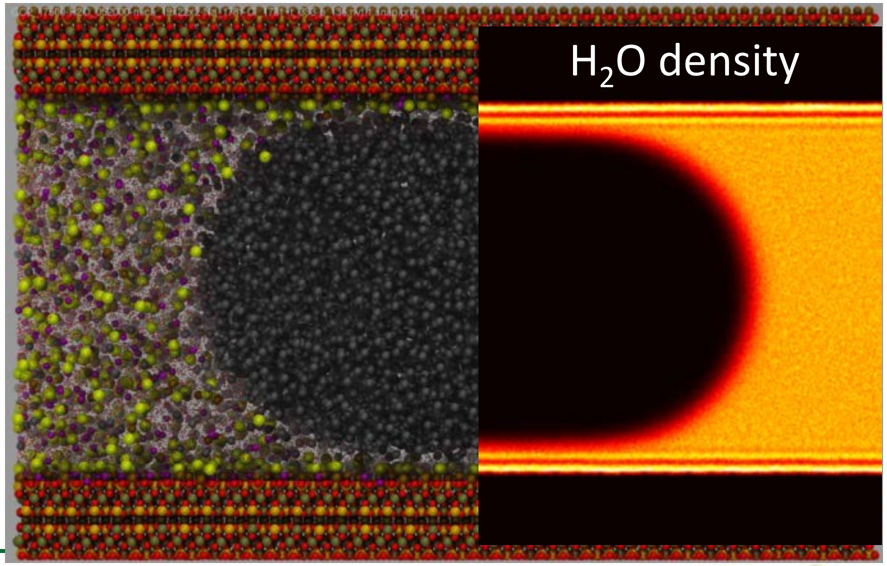
Understand the link between molecular-scale interactions and macroscopic wetting behavior for supercritical CO_2-brine-mineral systems.

Conclusions

Nanoscale distribution of dissolved species can vary significantly for different mineral surfaces, in spite of similar macroscopic contact angles.

Impact on Geological Carbon Storage

Because dissolution and precipitation of minerals depend strongly on the local distribution of CO_2, H_2O, and ion species, nanoscale surface interactions will influence long-term mineralization of injected carbon.



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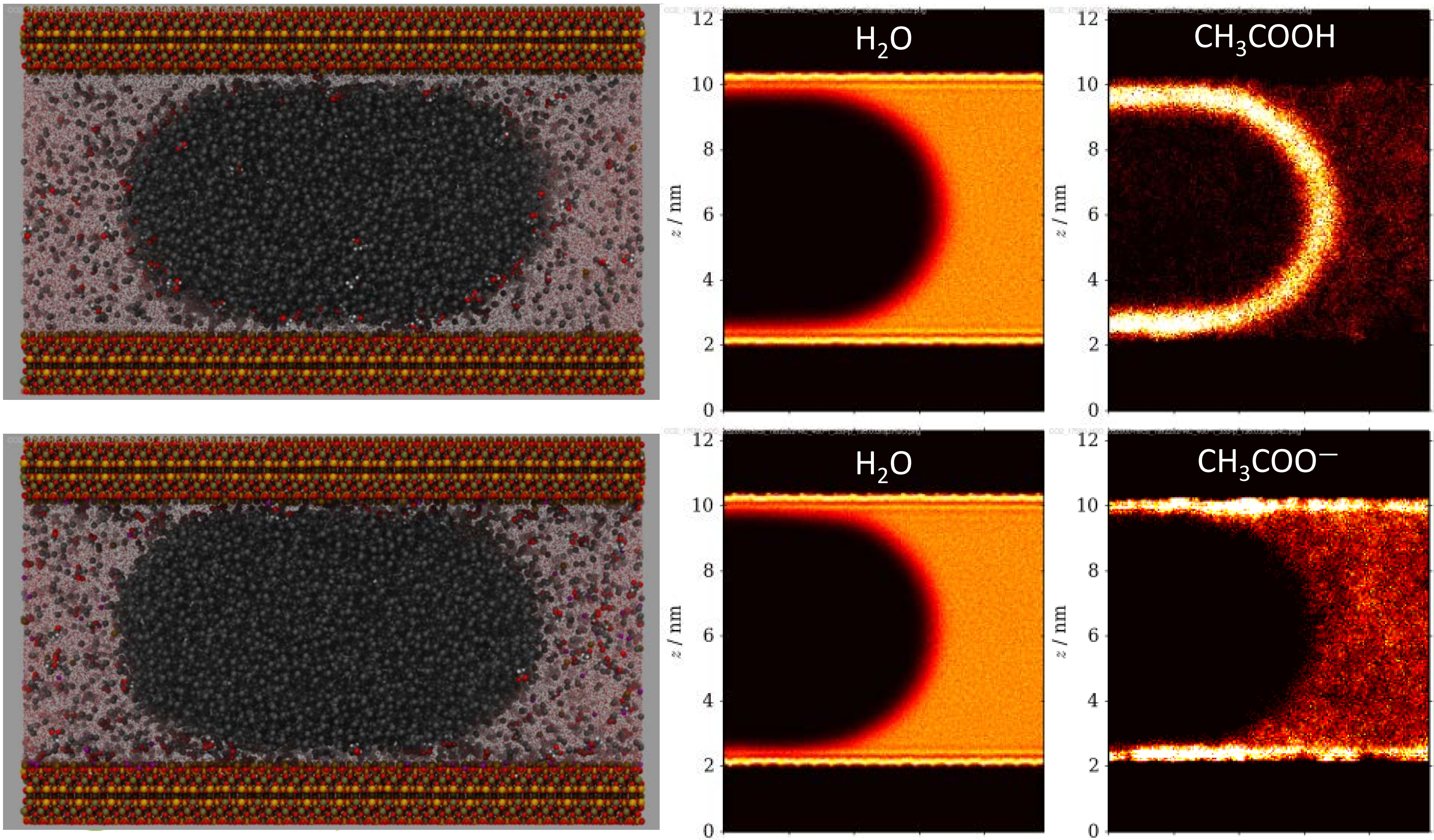
Example: pH alters interfacial partitioning



CO_2 Relative Permeability in Berea Sandstone

Research Team

Xiongyu Chen, Amir Kianinejad, David DiCarlo, and Gary Pope

Objectives of Research

Accurately measure CO_2 relative permeability in a CO_2 brine system in outcrop and reservoir rocks. Previous measurements by varying research groups showed a relative permeability a factor of ten lower than for other non-wetting phases.

Conclusions

We find that the CO_2 relative permeability is very close to that of other non-wetting phases. We used a longer (2' as opposed to 2") core and pressure taps to avoid end effects which are greater with a low viscosity fluid.

Impact on Geological Carbon Storage

Relative permeability is *the* crucial parameter for predicting fate, transport, and trapping of CO_2 on reservoir scales.

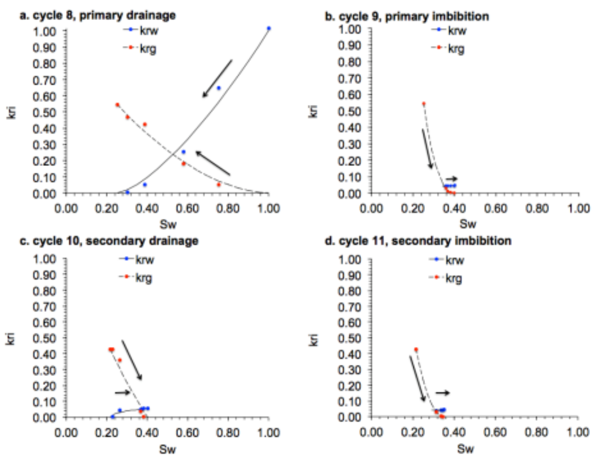


Figure 9. Relative permeability curve in Exp4: (a) primary drainage cycle; (b) primary imbibition cycle; (c) secondary drainage cycle; (d) secondary imbibition cycle.

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CO_2 Solubility in Saline Waters Containing SO_4^{2-}, Ca^{2+}, and HCO_3^-.

Research Team

Kim Gilbert with Phil Bennett

Objectives of Research

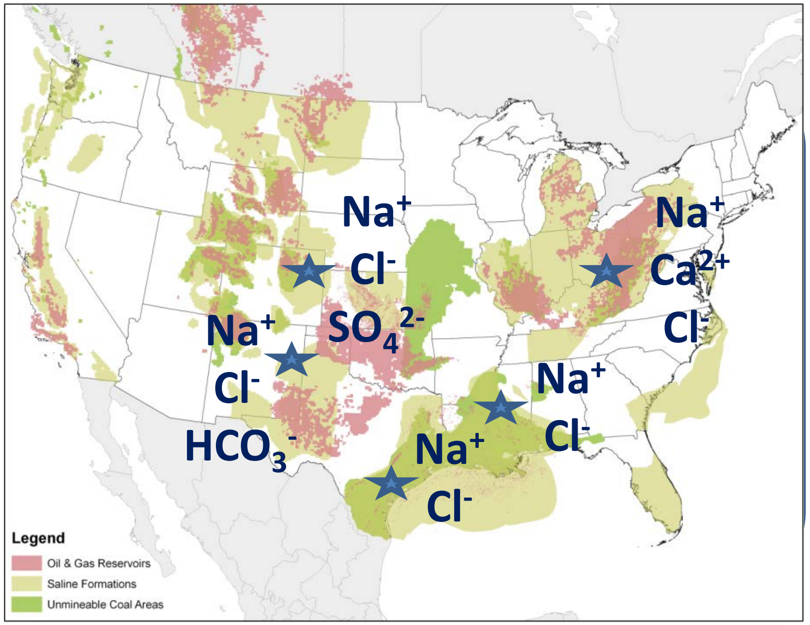
Understand brine-CO_2 interactions during a CO_2 injection

Conclusions

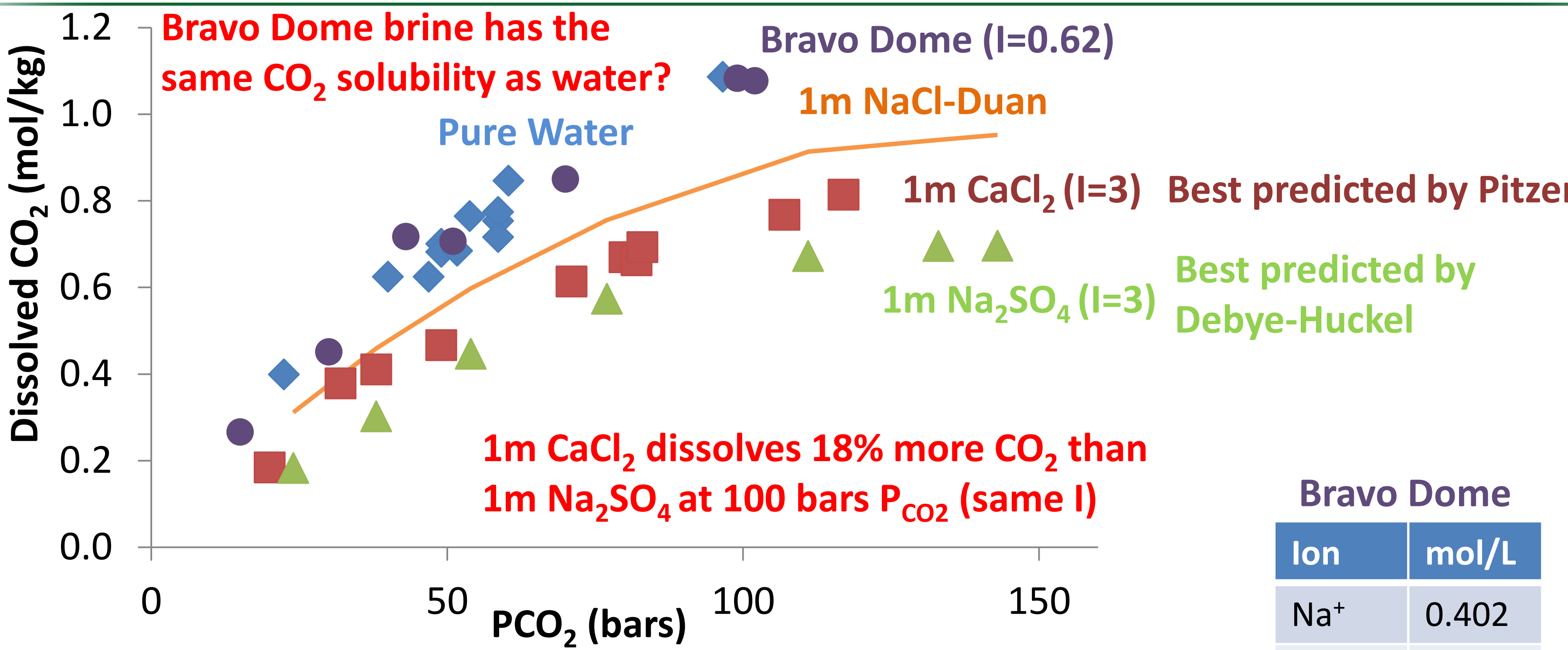
Ion complexation in SO_4^{2-} and HCO_3^- waters has significant effects on CO_2 solubility in ways that are not well predicted by models.

Impact on Geological Carbon Storage

The presence of SO_4^{2-} or HCO_3^- in a reservoir could cause an overestimate or underestimate in CO_2 solubility, respectively.



CO_2 Solubility in Brines – 57°C



Bravo Dome

Ion	mol/L
Na^+	0.402
Ca^{2+}	0.047
Cl^-	0.395
SO_4^{2-}	**0.024**
HCO_3^-	**0.101**

CONCLUSIONS

1. Ion type affects CO_2 solubility. Dissolved CO_2 predictability is improved by considering complexation.
2. Models under-predict CO_2 solubility in the presence of HCO_3^-.

Symbol size represents +/- 1 max st dev
Maximum standard deviation = 0.03 mol/kg

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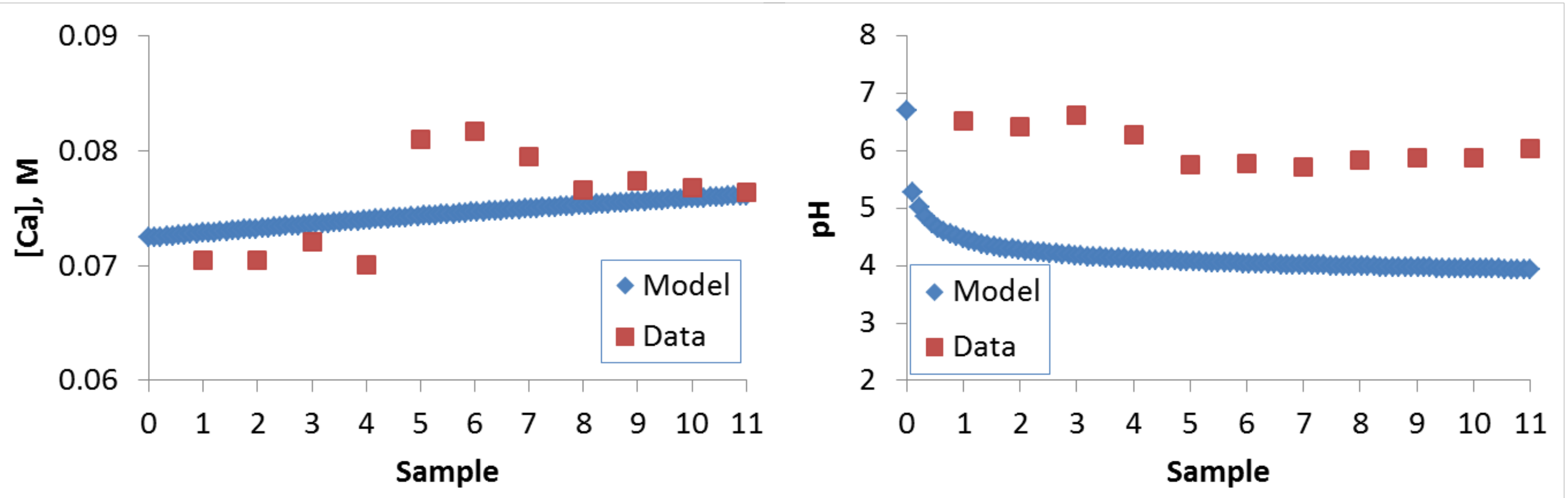
Mineral Dissolution and Precipitation during CO_2 Injection at the Frio-I Brine Pilot: Geochemical Modeling and Associated Uncertainties

Research Team

Anastasia Ilgen and Randall Cygan

Objectives of Research

1. Method development – incorporating Pitzer activity model
2. Geochemical modeling of calcite dissolution during Frio-I Pilot test
3. Uncertainties in calcite dissolution
4. Reactive flow modeling of mineral dissolution/precipitation over hundreds of years



Conclusions

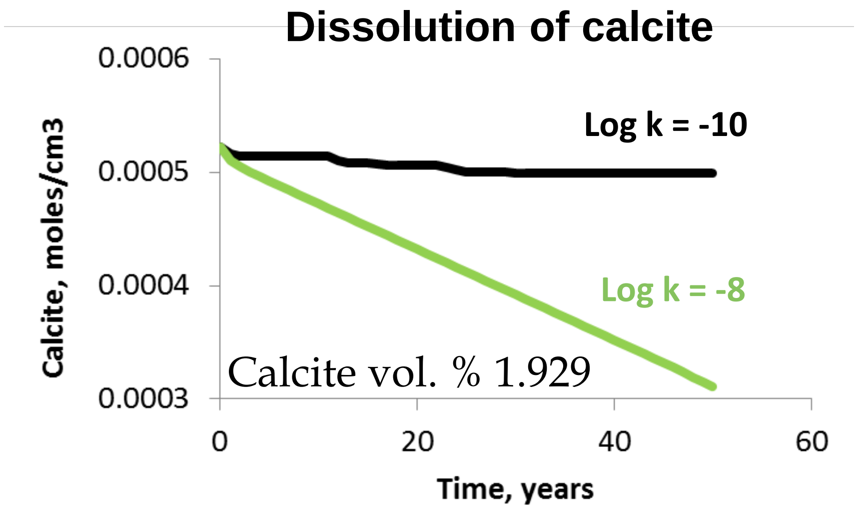
Model matches Ca^{2+} concentration; measured pH is significantly below predicted, possibly due to *ex situ* measurement conditions.

Mineral Dissolution and Precipitation during CO_2 Injection at the Frio-I Brine Pilot: Geochemical Modeling and Associated Uncertainties

Conclusions

<u>Uncertainty in calcite dissolution</u>: over 50 years differs by 60%

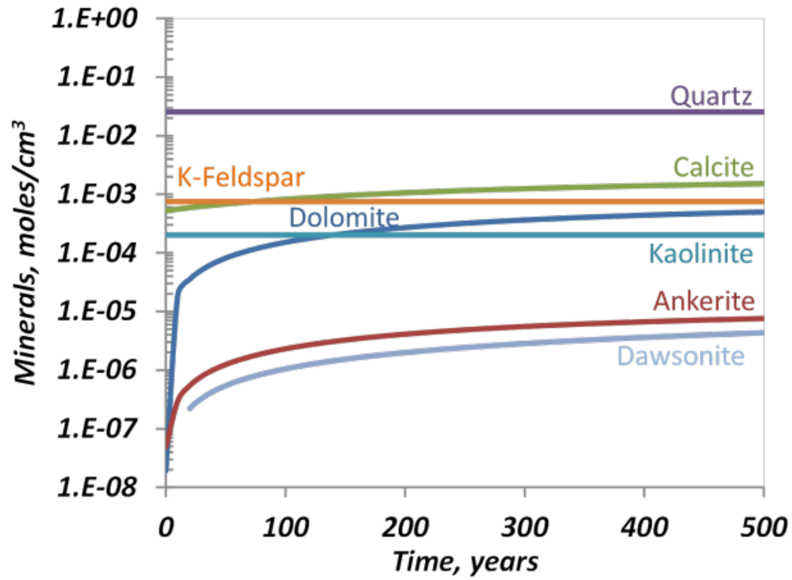
<u>Reactive Flow models</u>: As CO_2 is dispersed, carbonate mineral precipitation is predicted for time scale of >10 years. Calcite is the most abundant, significant precipitation of dolomite and ankerite.



Impact on Geological Carbon Storage

Further interpretation of the Frio-I test data: comparison between calcite dissolution observed in the field and the geochemical model outcome

Quantification of uncertainty during geochemical modeling of calcite dissolution



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Estimation of Arrival Times of Phases in Acoustic Emissions

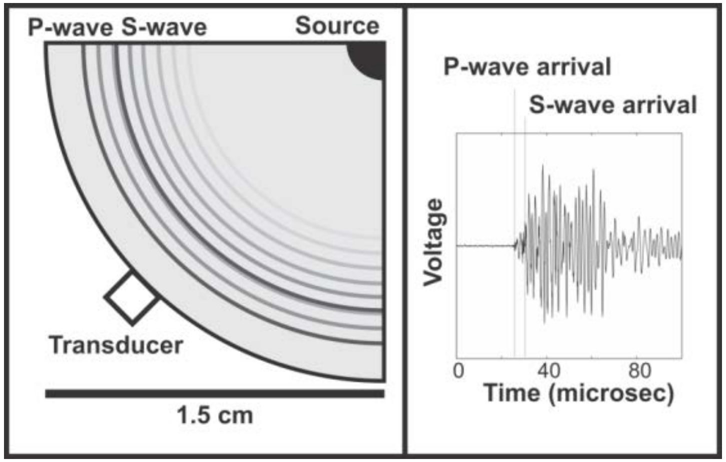
Research Team

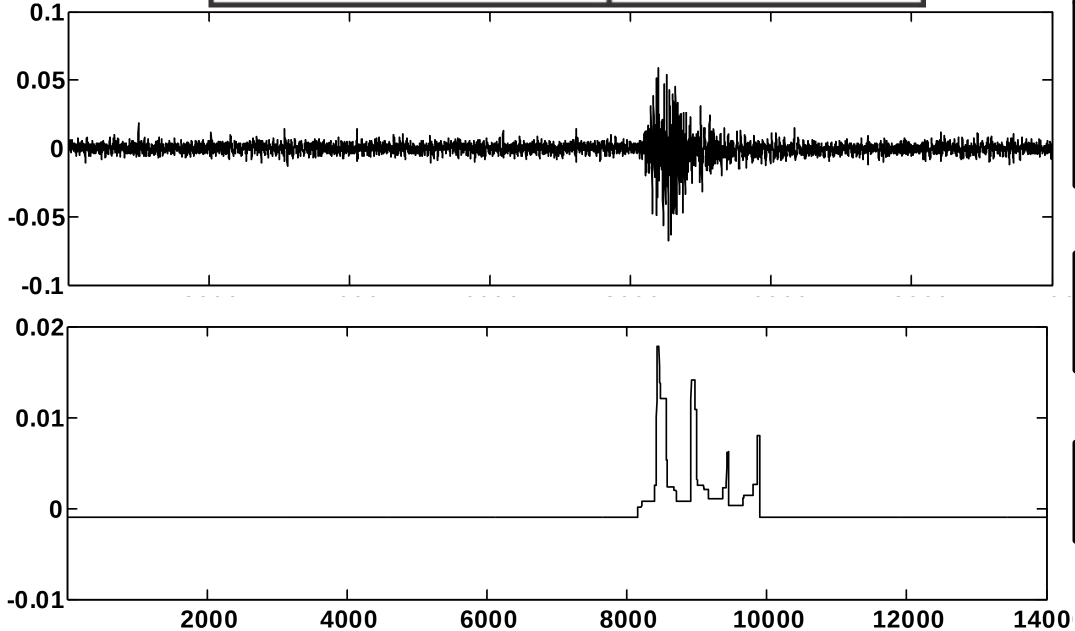
Alex Rinehart, Sean McKenna, and Thomas Dewers

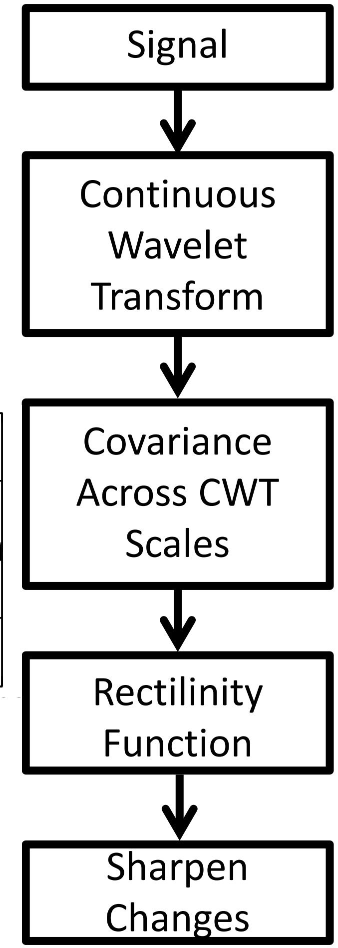
Objectives of Research

Rapid automated picking of P- and S-waves in AE as-good-as manual.

Better characterize damage in small-sized experiments.







Estimation of Arrival Times of Phases in Acoustic Emissions

Conclusions

Basic filtering designed.

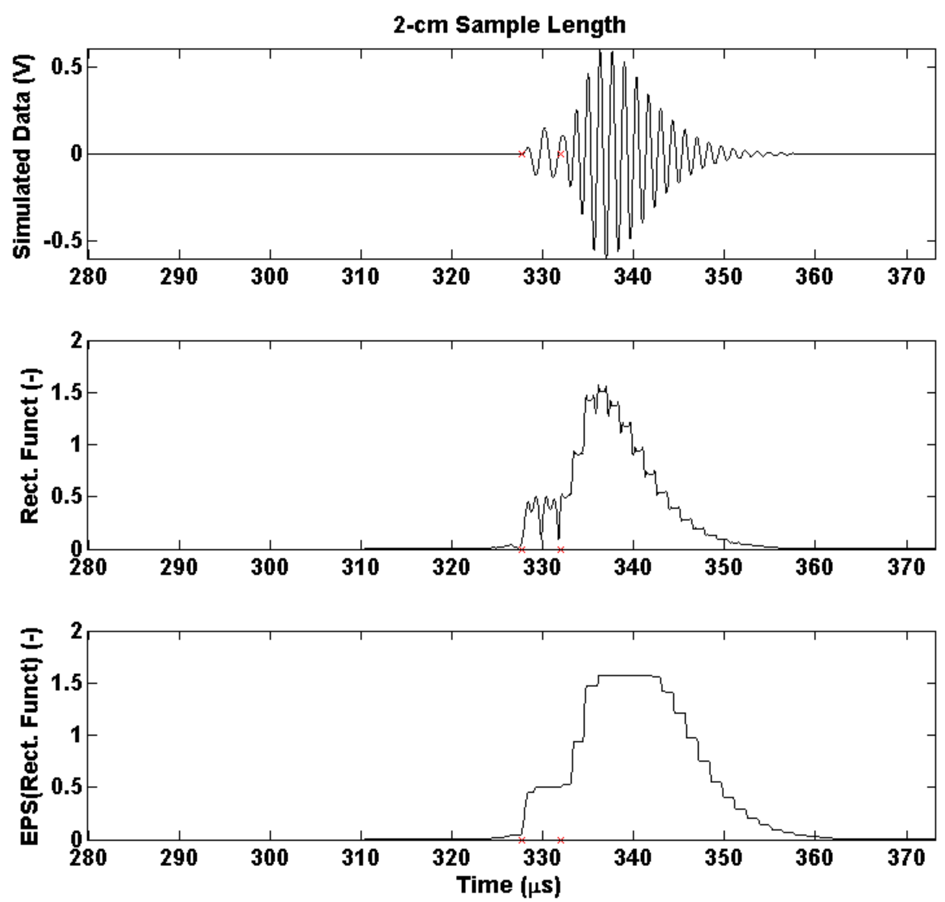
'Good-as-manual'.

Specific details of picking in progress.

Impact on GCS

Increase detail of laboratory rock damage measurements.

Extensions to single-component seismographs and logging possible.



Upscaling of reactive transport model from pore to continuum scale using a response function approach

Research Team

Hongkyu Yoon, Bill Arnold, and Tom Dewers

Objectives of Research

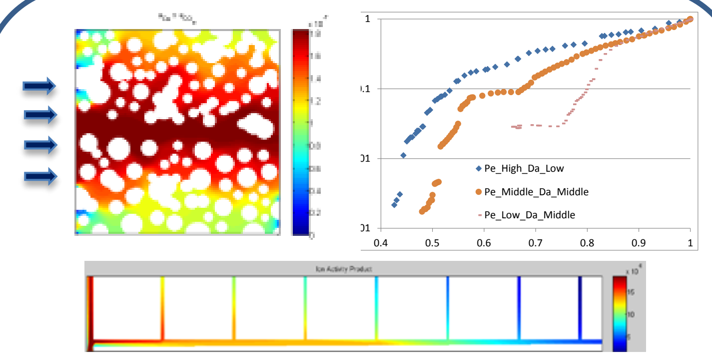
Develop a response function approach to upscale the reactive transport processes from the pore to continuum scales

Conclusions

Hybrid pore-scale reactive transport (RT) model is used to calculate changes in the critical pore-scale relationships necessary for accurate continuum scale reactive transport modeling and construct the response function of relationships. Continuum RT model with response functions is used to calculate changes in fault-zone permeability

Impact on Geological Carbon Storage

- Competing hypotheses based on experimental and field observations of cementation are tested by high-fidelity pore-scale simulation and upscaled continuum scale RT model
- Significant improvement of risk assessment of CO_2 leakage pathway through fault sealing



Pore structure (left) used to develop permeability-porosity relationships under different Pe-Da regimes (right). Fracture network with varying apertures is used to mimic travertine patterns at Crystal Geyser

Some Insights into the Scale up of Reactive-Diffusive Processes in Heterogeneous Media

Research Team

Harpreet Singh, Saeed Oveyasi, Sanjay Srinivasan

Objectives of Research

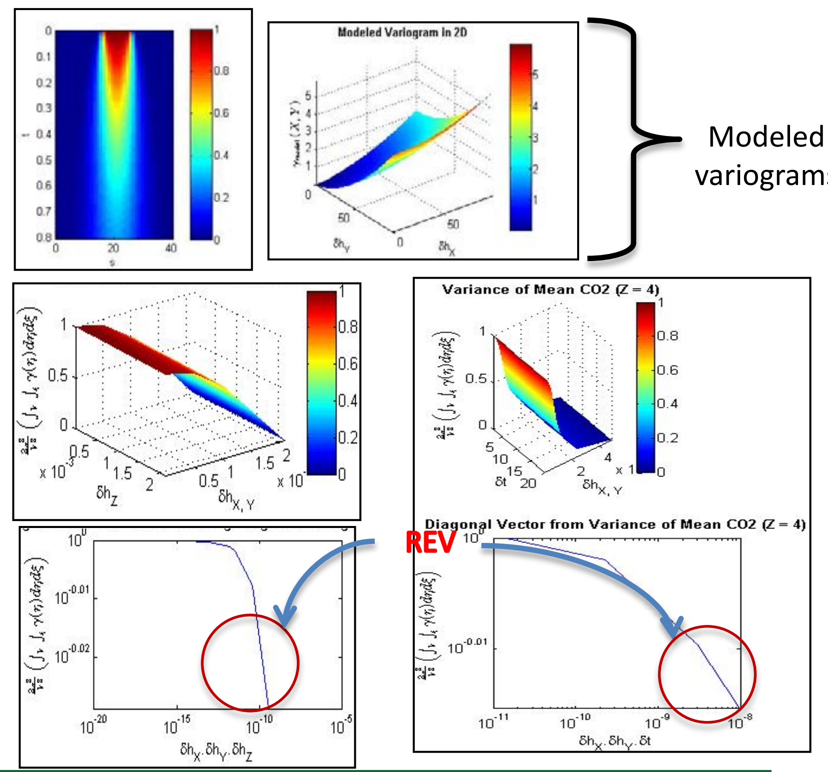
- Investigate scaling (spatiotemporal) behavior of reactive transport in heterogeneous media
- Propose general methodologies that can be used to predict scale-appropriate behavior

Conclusions

- Semi-analytical scale-up based on a perturbation solution of the Advection-Diffusion-Reaction equation reveals that heterogeneity plays a major role in definition of effective mixing zone length and dispersion coefficient

Impact on Geological Carbon Storage

- Analysis revealed change in REV due to pore structure alteration in a reactive process
- Important implications regarding selection of spatial and temporal descretizations in numerical models for such processes



Results From the Scale-Up Analysis of Pore Scale Experimental Data

Research Team

Sanjay Srinivasan, Saeed Oveyasi, Harpreet Singh

Objectives of Research

Perform scale up analysis of calcite concentration data from lab measured pore scale models for both reactive and non-reactive cases

Determine how reactions changes estimates for spatiotemporal REV

Conclusions

Change in REV due to pore structure alteration in a reactive process

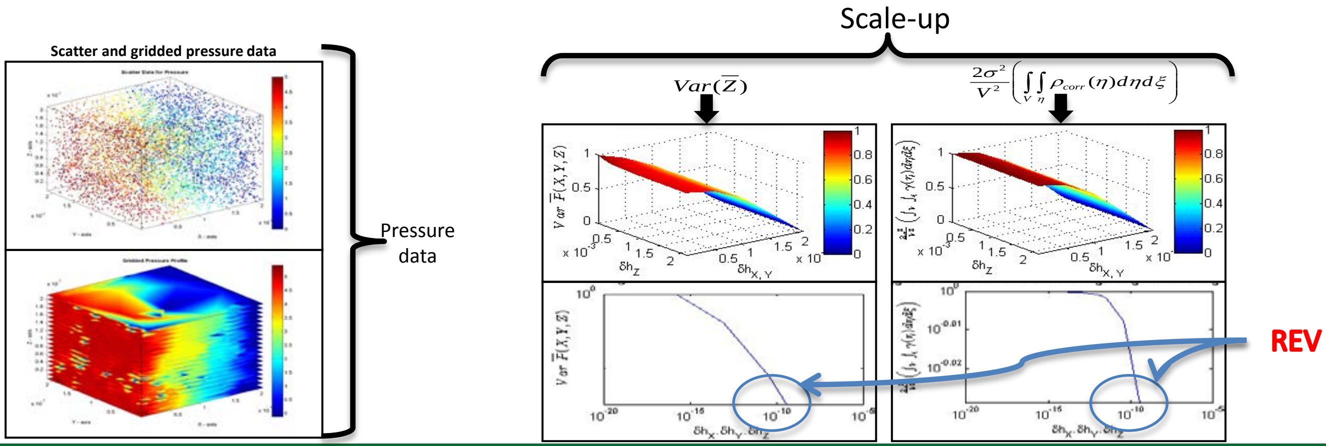
Reactions tend to stabilize the spatiotemporal covariance of concentrations

Impact on Geological Carbon Storage

Reactive processes are highly sensitive to scale-dependence (in space and time).

Important implications in engineering field-scale geological storage of CO_2

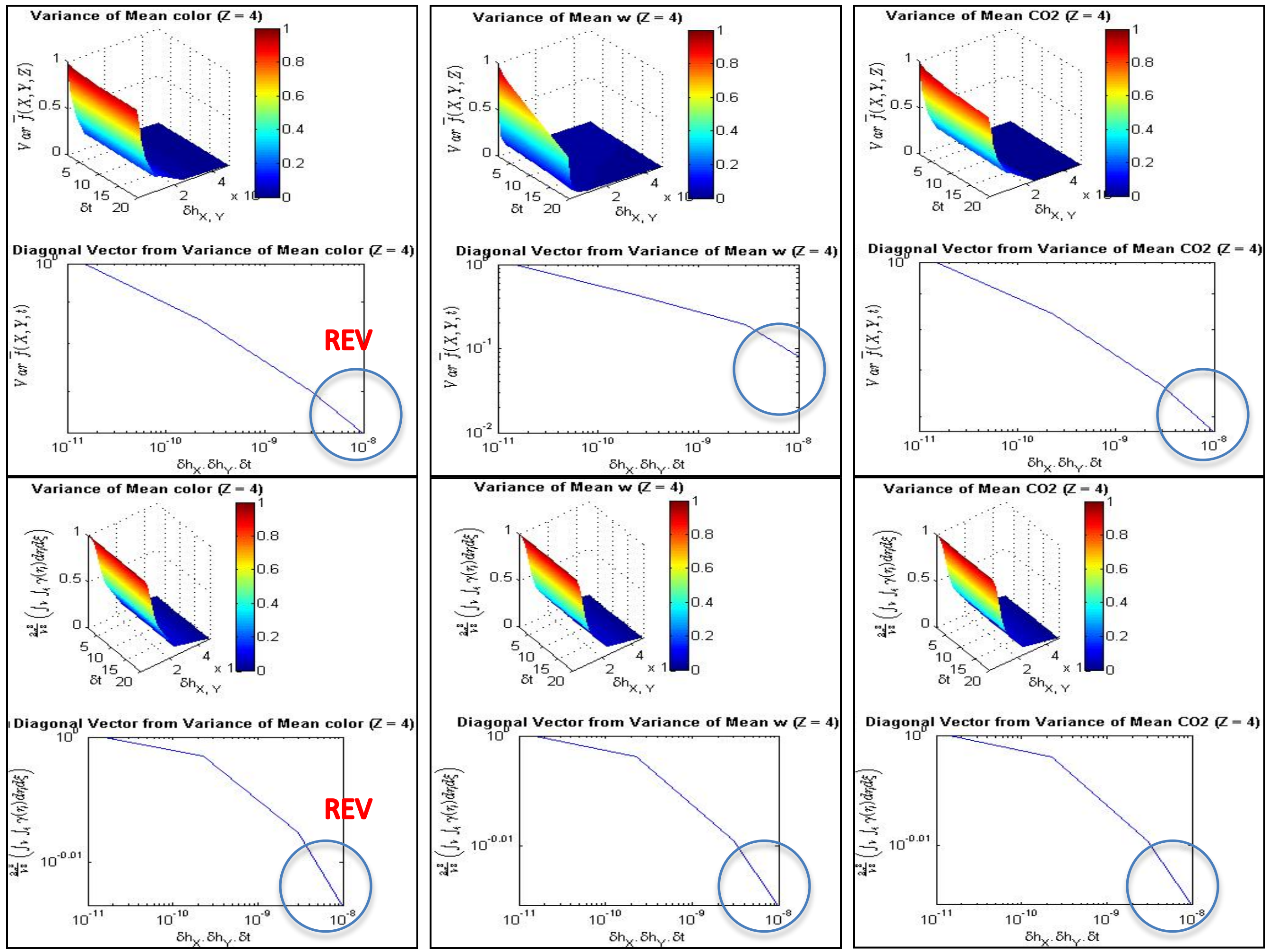
NONREACTIVE PROCESS: SCALE-UP



Reactive Process: Scale-up

$$Var(\overline{Z})$$

$$\frac{2\sigma^2}{V^2}\left(\int_V\int_\eta \rho_{corr}(\eta)d\eta d\xi\right)$$



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New models for flow and transport through fractures

Research Team

Philip Bennett, Bayani Cardenas, Lichun Wang

Objectives of Research

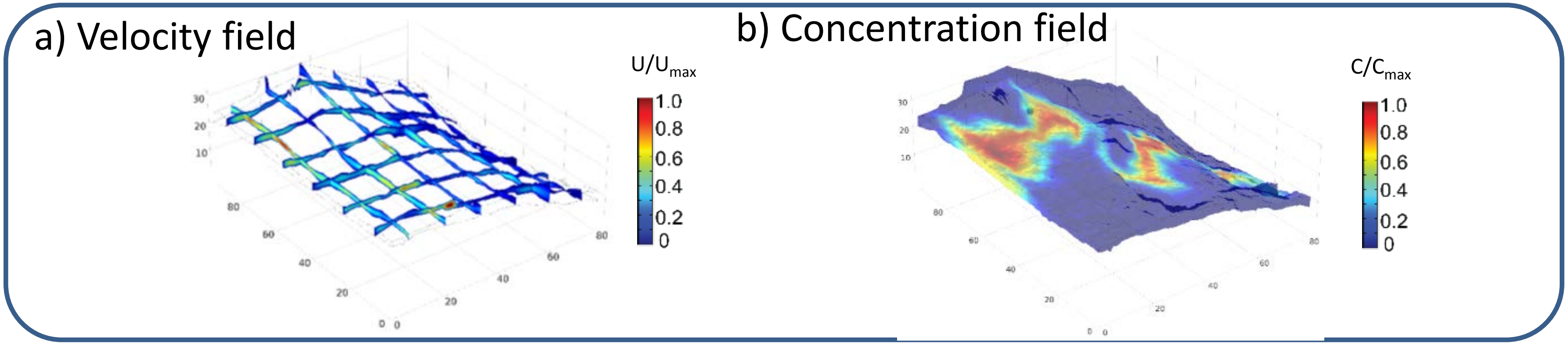
To develop models that accurately and efficiently quantify hydraulic and transport parameters based on the geometric properties of discrete fractures.

Conclusions

The new Generalized Cubic Law can accurate capture the local fluid process, and thus can be further applied to predict the effective transport properties of discrete fractures.

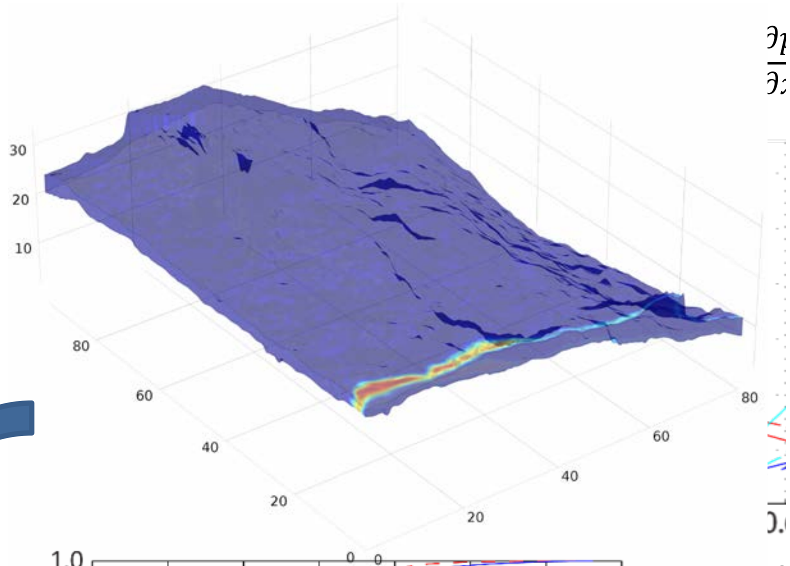
Impact on Geological Carbon Storage

The estimated parameters can be readily used in discrete fracture network model used to predict large-scale SC-CO_2-related transport phenomenon

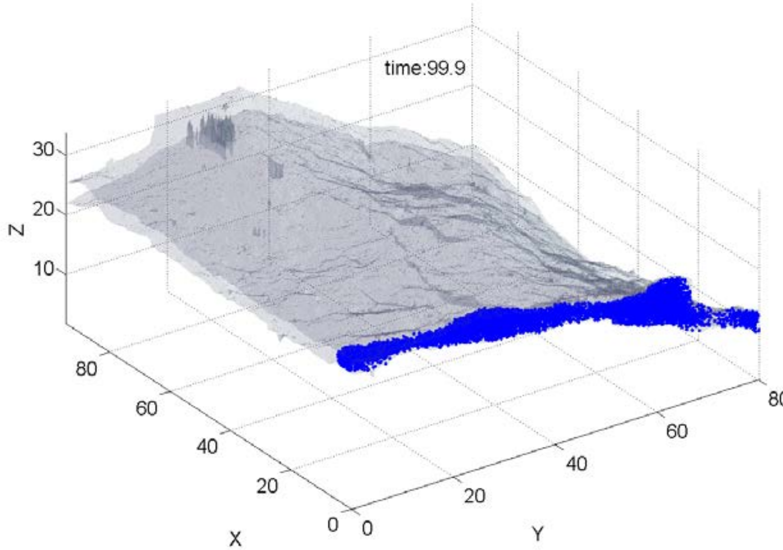


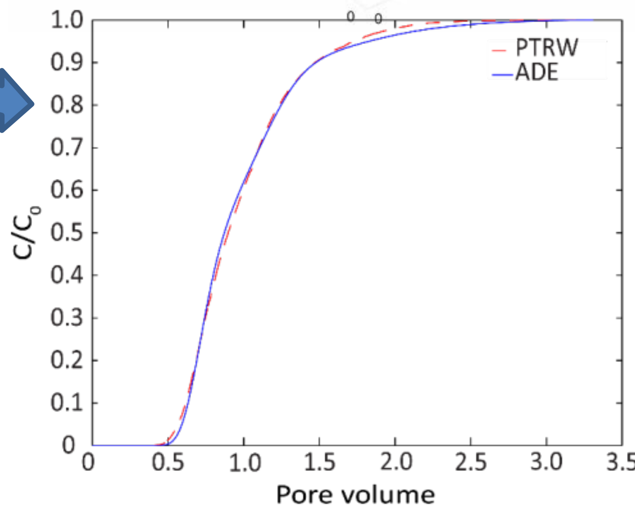
New models for flow and transport through fractures

Advection-Diffusion-Equation



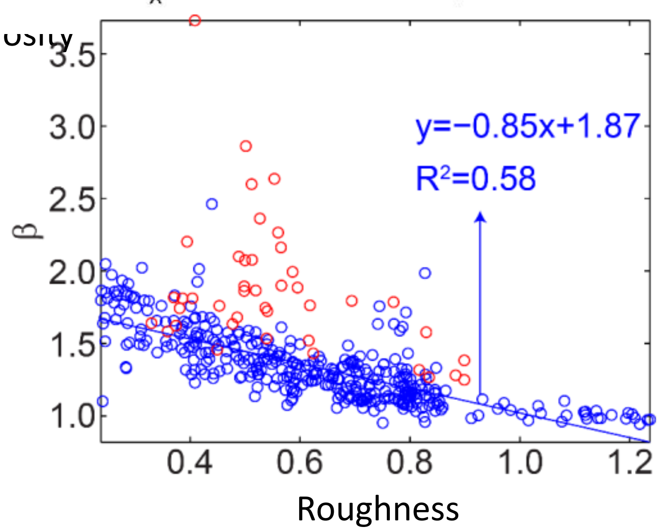
Particle Tracking Random Walk





Non-Fickian breakthrough curves

CTRW model



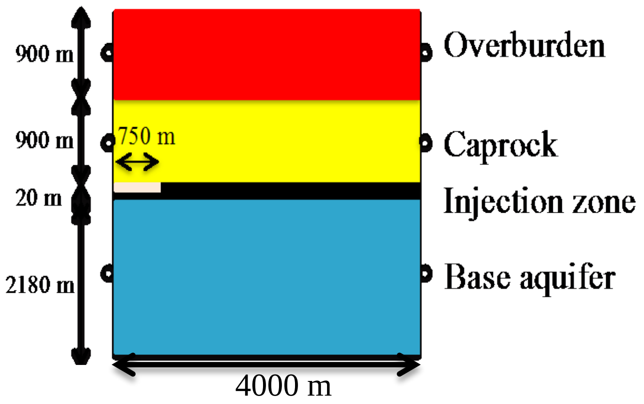
Sensitivity analysis on InSalah

Research Team

P. Newell, H. Yoon, M.J. Martinez, B.E. Bishop and S.E Bryant

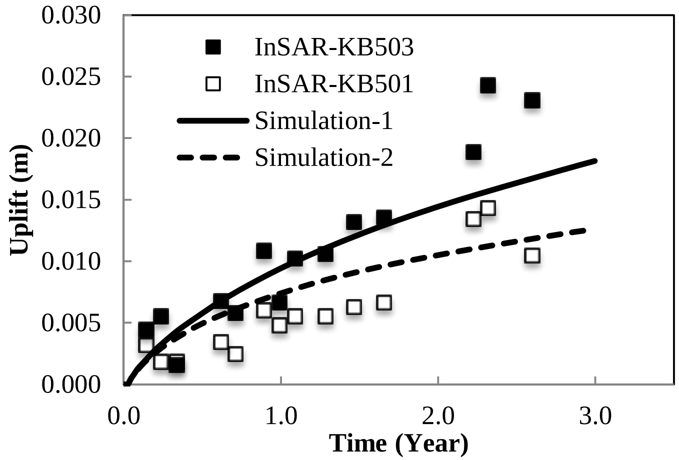
Objectives of Research

- **Validate our coupled geomechanical model.**
- **Sensitivity analysis as well as model calibration.**



Conclusions

- **The model can accurately predict the uplift for KB-501 and KB-503 measured by using best-available (but uncertain) material properties.**
- **The uplifts are highly sensitive to both hydrogeological and geomechanical properties.**



Impact on Geological Carbon Storage

- **Better understanding of the reservoir's dynamics.**
- **Quantifying the impact of the engineering and geological assumptions on reservoir's behavior.**
- **Identifying the important uncertain parameters.**

Constraints on the Magnitude and Dissolution of CO_2 at Bravo Dome Natural Gas Field

Research Team

Kiran Sathaye, Marc Hesse

Danny Stockli and Martin Cassidy

Objectives of Research

Determine age of magmatic CO_2 at Bravo Dome

Compute amount dissolved since emplacement

Conclusions

CO_2 entered 1.2 to 1.5 million years ago

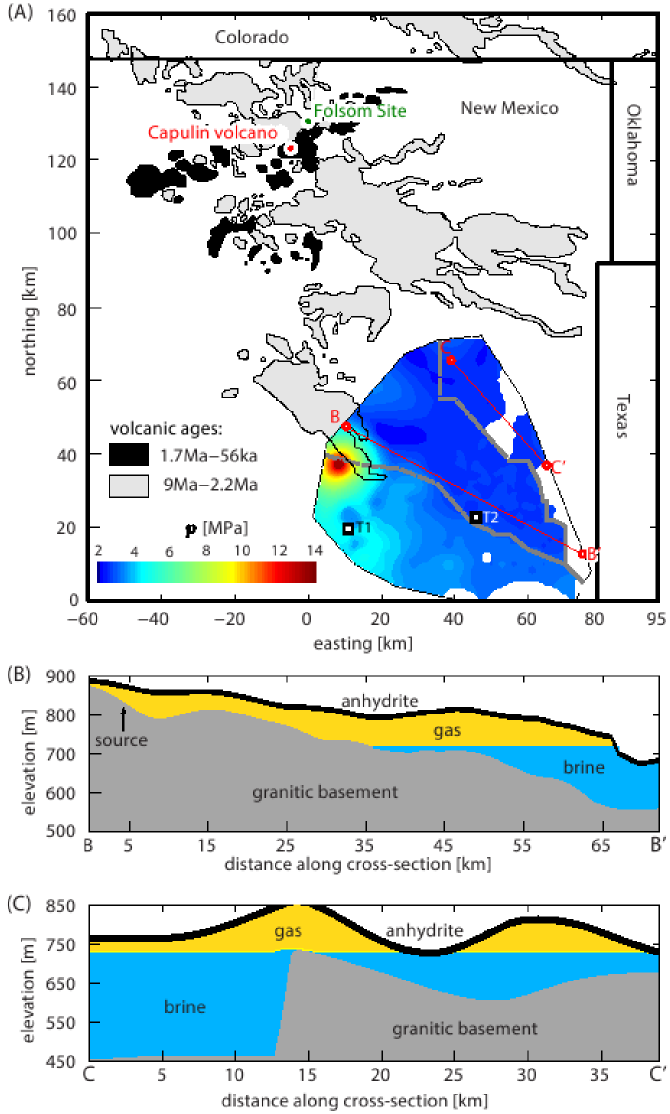
22% has dissolved

Impact on Geological Carbon Storage

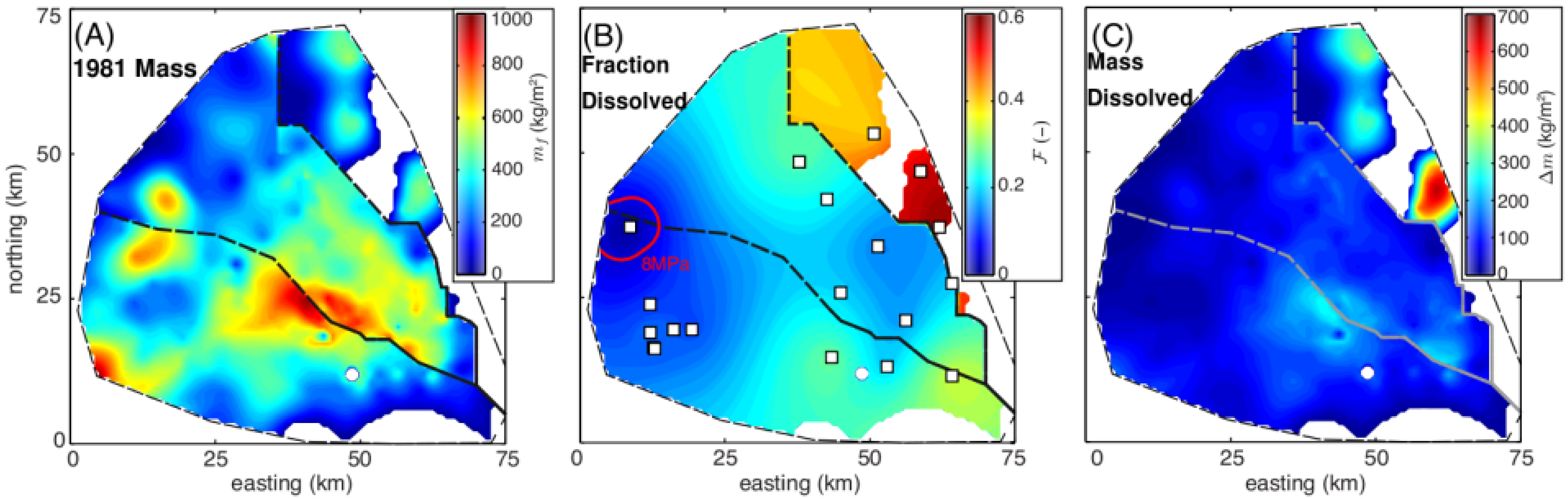
Previous age estimate was as young as 10,000 years

Only 360Mt CO_2 dissolved over 1.5Ma

Solubility trapping in typical saline aquifers may not be a significant process for securing CO_2



Total Dissolution Calculation



- Total 1981 mass: 1.3±0.6GtCO_2
- Total original mass: 1.6±0.7GtCO_2
- Mass loss: 366±120MtCO_2 (22±7% dissolved)
- 40% of dissolution into residual brine in gas layer
- 366Mt ≈ 75 years of 1 coal power plant emissions

Impact of Capillary Transition Zone on CO_2 Dissolution Into Brine

Research Team

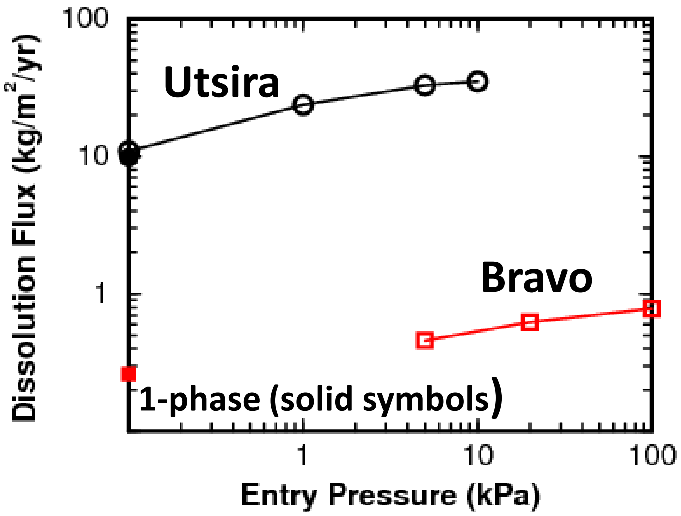
Mario J. Martinez & Marc A. Hesse

Objectives of Research

Determine the influence of the capillary "fringe" region on the convectively driven dissolution of CO_2 in brine:

- **Long-term quasi-steady dissolution flux**
- **Onset time**

Dissolution Flux vs. Entry Pressure



Conclusions

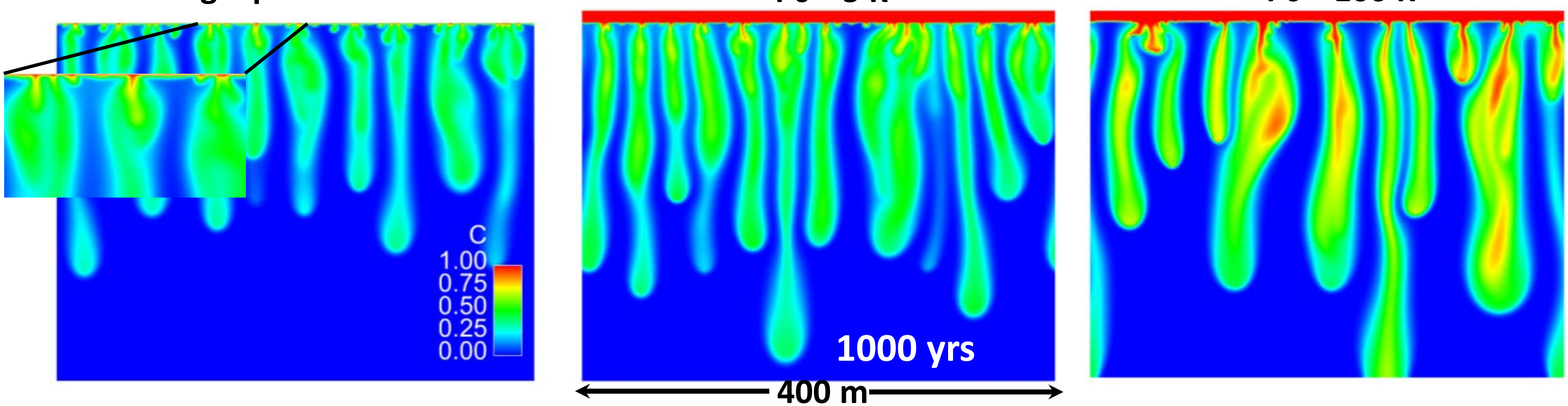
The quasi-steady convectively driven dissolution flux increases and the onset time decreases when the capillary fringe is included in the analysis.

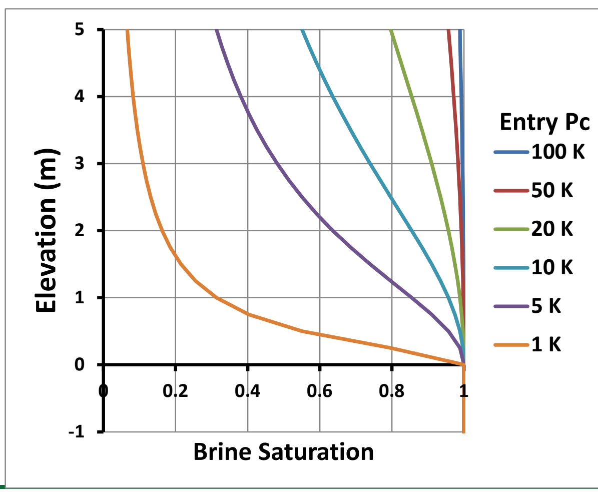
Impact on Geological Carbon Storage

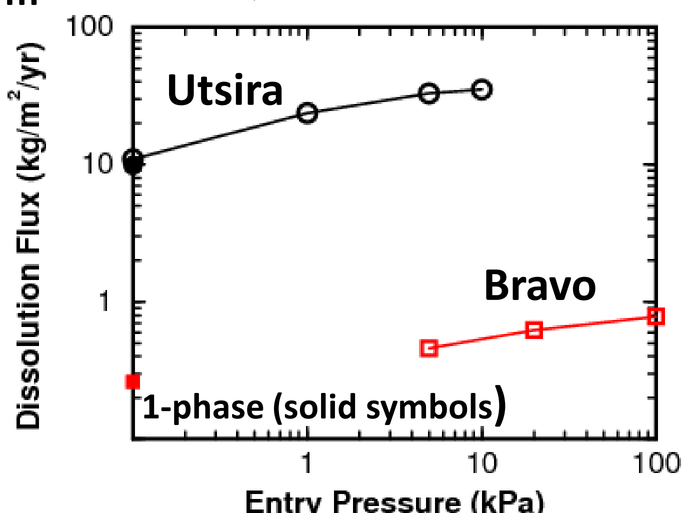
Convectively driven dissolution flux may be roughly 3x larger than current estimates which ignore the capillary transition region.

Impact of Capillary Transition Zone on CO_2 Dissolution Into Brine

Dissolved CO_2 in Reservoir similar to Bravo Dome
(k= 50 mD poro = 0.15)







Impacts of Reservoir Heterogeneity on CO_2 Injection at Bravo Dome

Research Team

Bill Arnold

Objectives of Research

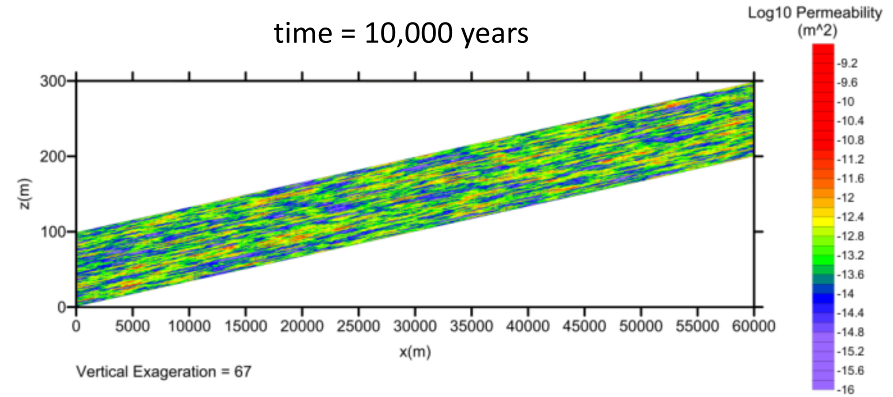
Evaluate increased CO_2 dissolution caused by isolated bodies of brine resulting from reservoir heterogeneity during filling

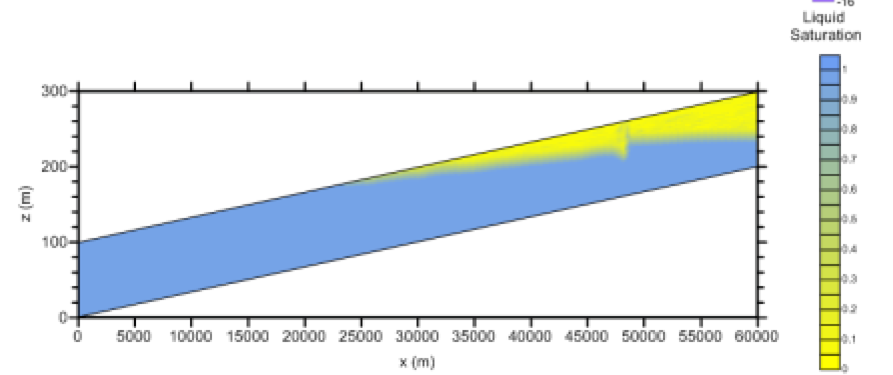
Conclusions

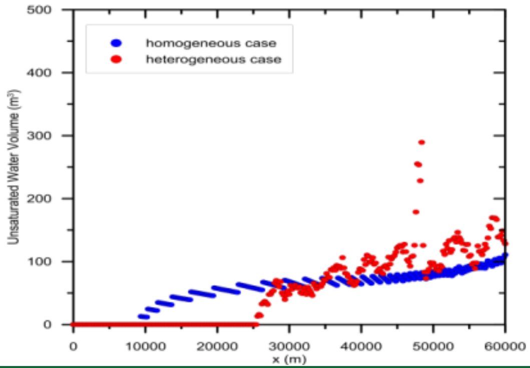
Preliminary simulations indicate filling time for the reservoir on the scale of tens of thousands of years to avoid overpressures that would have disrupted the cap rock. Heterogeneity increases contact between liquid and gas phases and potential for dissolution, but not dramatically because of relatively slow filling process.

Impact on Geological Carbon Storage

Bravo Dome may have experienced less dissolution enhanced by heterogeneity than a CO_2 sequestration system because of relatively slow filling process







Isolation and Characterization of a Novel CO_2-Tolerant *Lactobacillus* Strain from Crystal Geyser, Utah, USA

Research Team

Eugenio F. U. Santillan (Jay), Phil Bennett

Objectives of Research

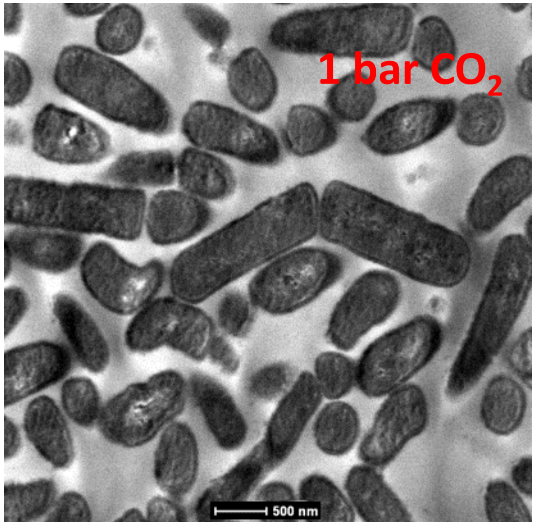
Determine the presence and viability of microorganisms in CO_2 rich environments

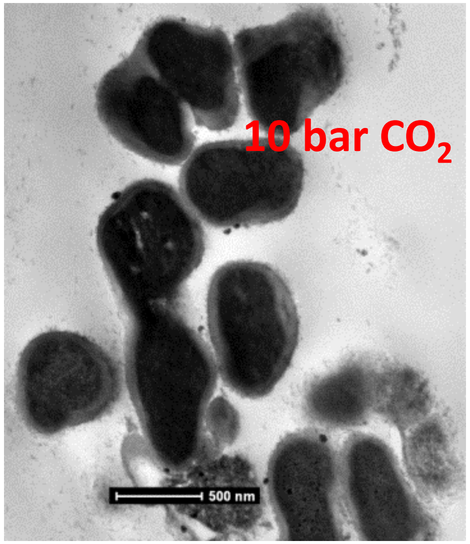
Conclusions

- Microbial communities exist in CO_2 rich environments and their composition is controlled by environmental variables in addition to CO_2
- First known hyper-capnophile (CO_2 loving organism) was isolated
  - Isolate is a fermenter, related to *Lactobacillus casei*
  - Grows up to 10 bar CO_2 and survives up to 25 bar
  - Indicates viability of microbial communities at high PCO_2

Impact on Geological Carbon Storage

Viable communities highlight microbes in CO_2 sequestration can affect geochemistry and permeability

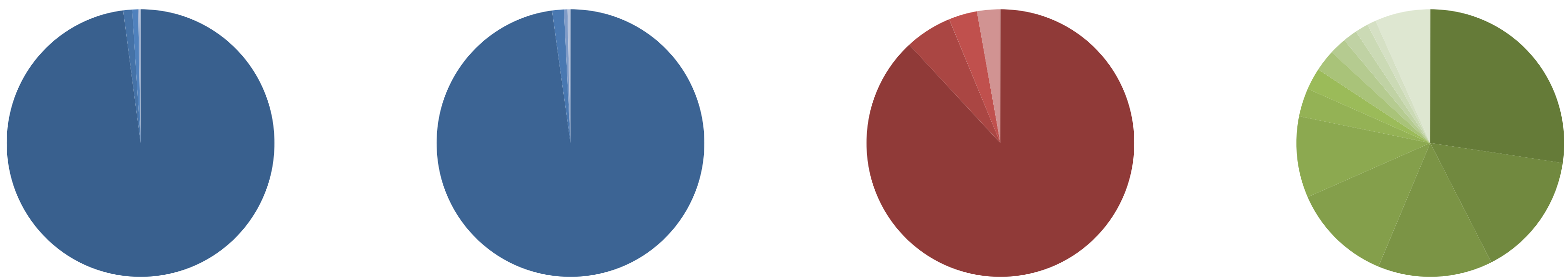


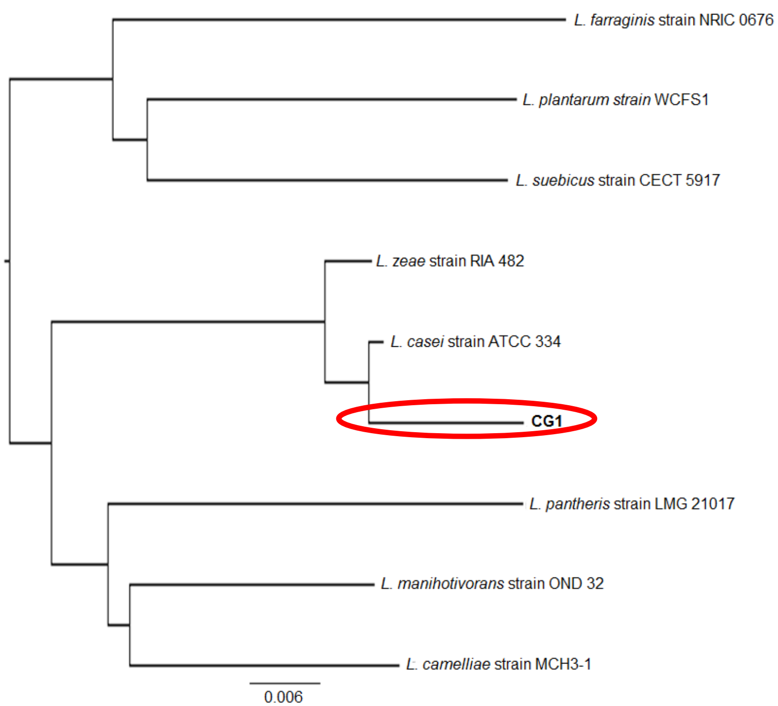


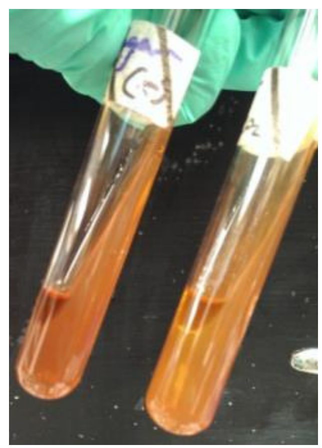
(Santillan et al *submitted*)

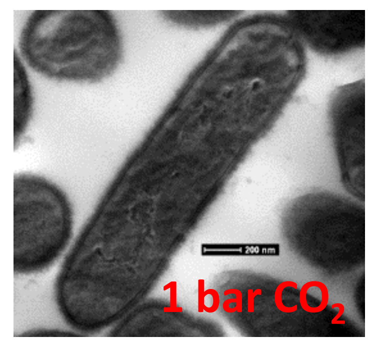
Isolation and Characterization of a Novel CO_2-Tolerant *Lactobacillus* Strain from Crystal Geyser, Utah, USA

Crystal Geyser | **Airport Spring** | **Bravo Dome** | **Klickitat**









(Santillan et al *submitted*)

Effect of CO_2-related alteration on fracturing of reservoir and seal rocks from the Crystal Geyser analog

Research Team

Jonathan Major, Peter Eichhubl, Tom Dewers

Objectives of Research

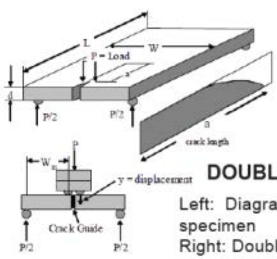
Measure geomechanical failure parameters (fracture testing) of naturally CO_2-altered rocks from the Crystal Geyser field site

Conclusions

CO_2-related alteration has a measurable impact on the fracture mechanical properties of reservoir and seal rocks, generally leaving them more prone to fracturing

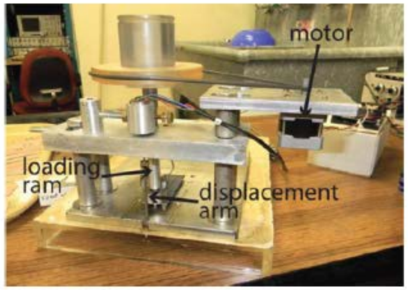
Impact on Geological Carbon Storage

1. Fractures are potential leakage pathways.
2. Differences in fracture mechanical properties affect growth of new fractures, fracture connectivity, spacing, clustering, and fracture network geometry, and thus leakage pathway geometry.

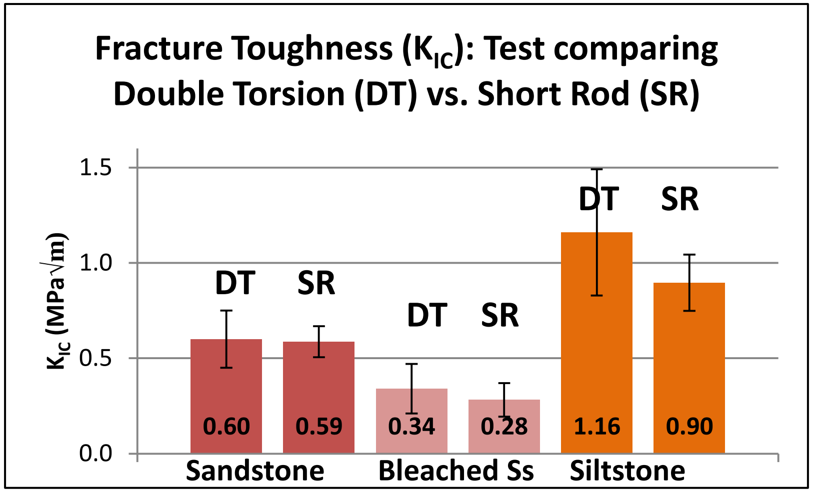


DOUBLE TORSION

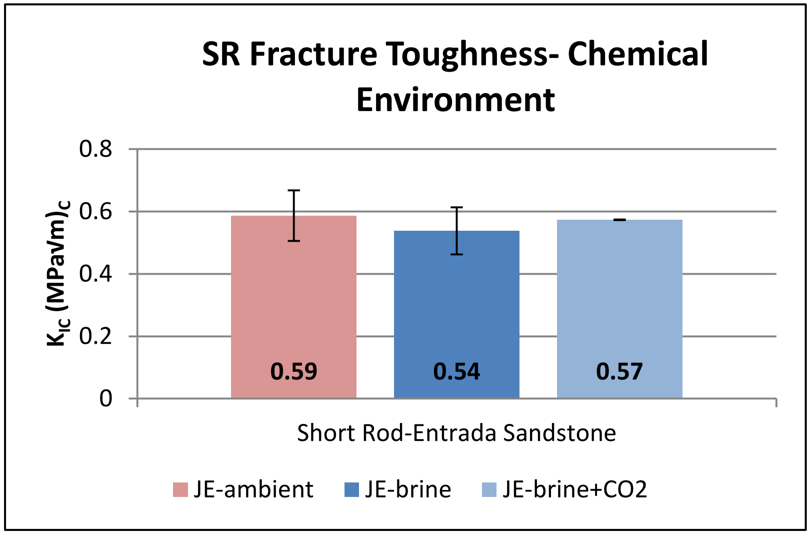
Left: Diagram of DT test specimen
Right: Double torsion test apparatus, UT-Austin CPE (from Fidler, 2011)



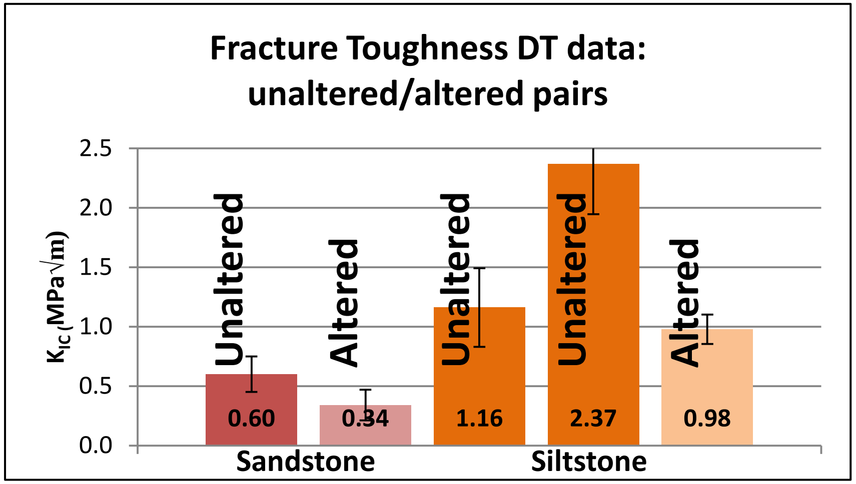
Effect of CO_2-related alteration on fracturing of reservoir and seal rocks from the Crystal Geyser analog

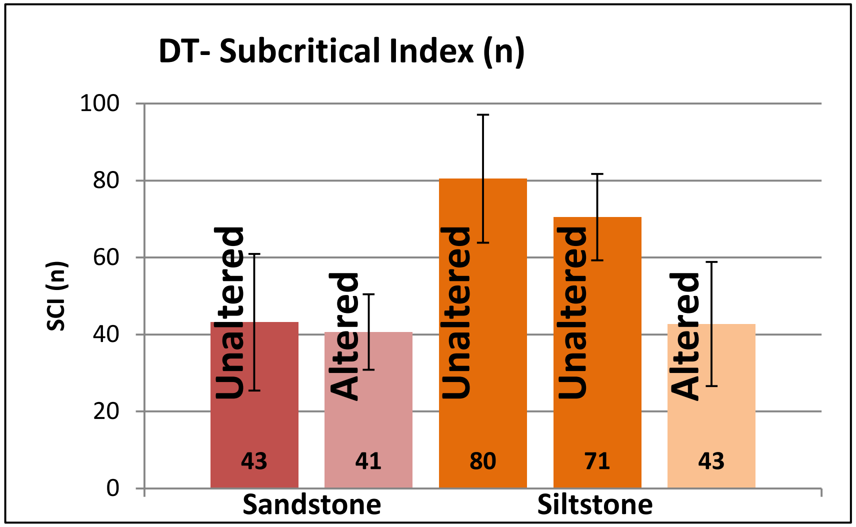


2 different test methods with different sample geometries yield comparable results



No measurable impact on fracture toughness





Fracture mechanical properties vary by altered/unaltered states, lithology

Seal capacity of CO_2-altered caprock from Crystal Geyser

Research Team

Jonathan Major, Peter Eichhubl

Objectives of Research

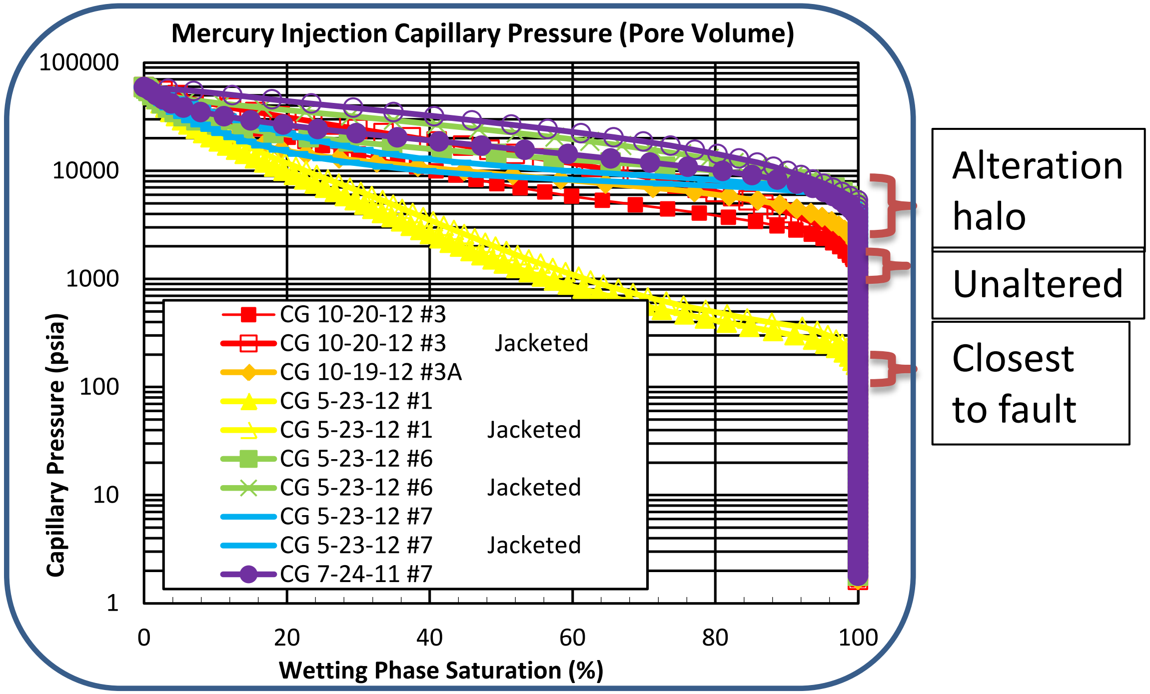
Assess seal capacity of CO_2-altered caprock from Crystal Geyser site

Conclusions

CO_2-related alteration impacts capillary behavior & CO_2 seal capacity of caprock

Impact on Geological Carbon Storage

1. **CO_2-related alteration has effect on caprock capillary seal capacity.**
2. **Lowering of seal capacity may control leakage in the absence of fractures.**



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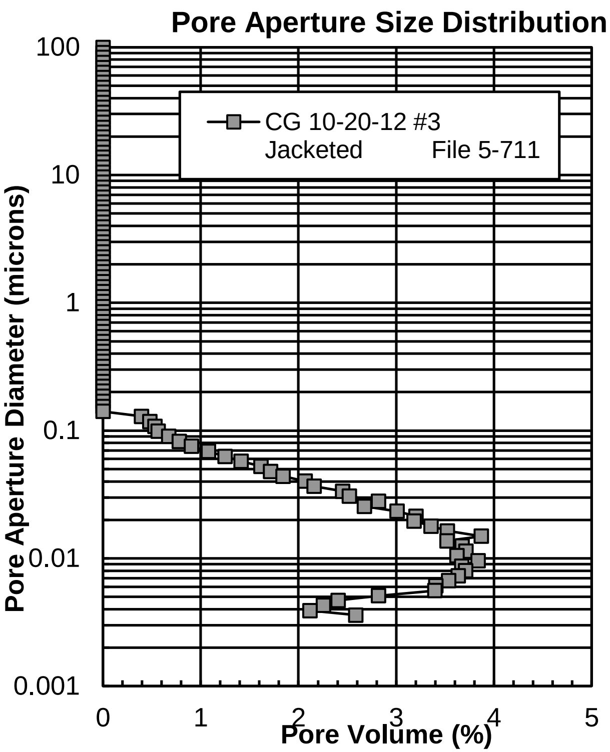
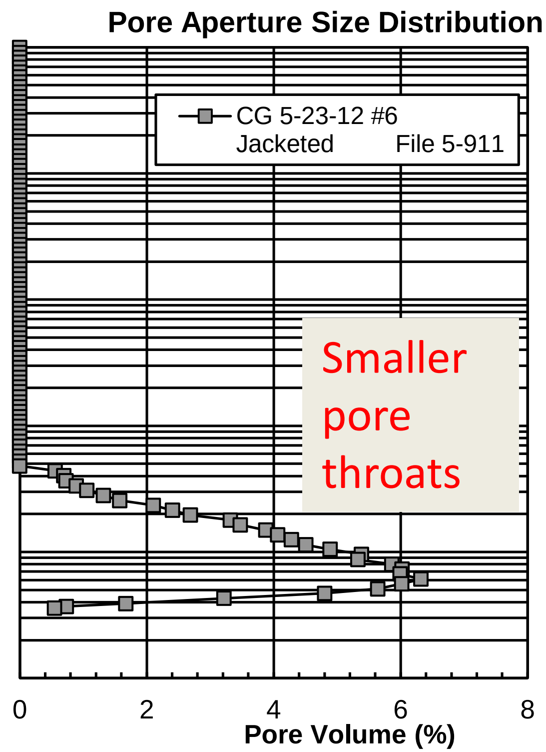
Seal capacity of CO_2-altered caprock from Crystal Geyser

- **Systematic trends seem to emerge, likely related to bulk mineralogical changes**
  - Calcite precipitation may be clogging up pore throats

Mancos Shale "background" (~5 wt% calcite)



Mancos Shale in alteration halo (~74 wt% calcite)



Mancos Shale at LGW fault, near seep (~48 wt% calcite)