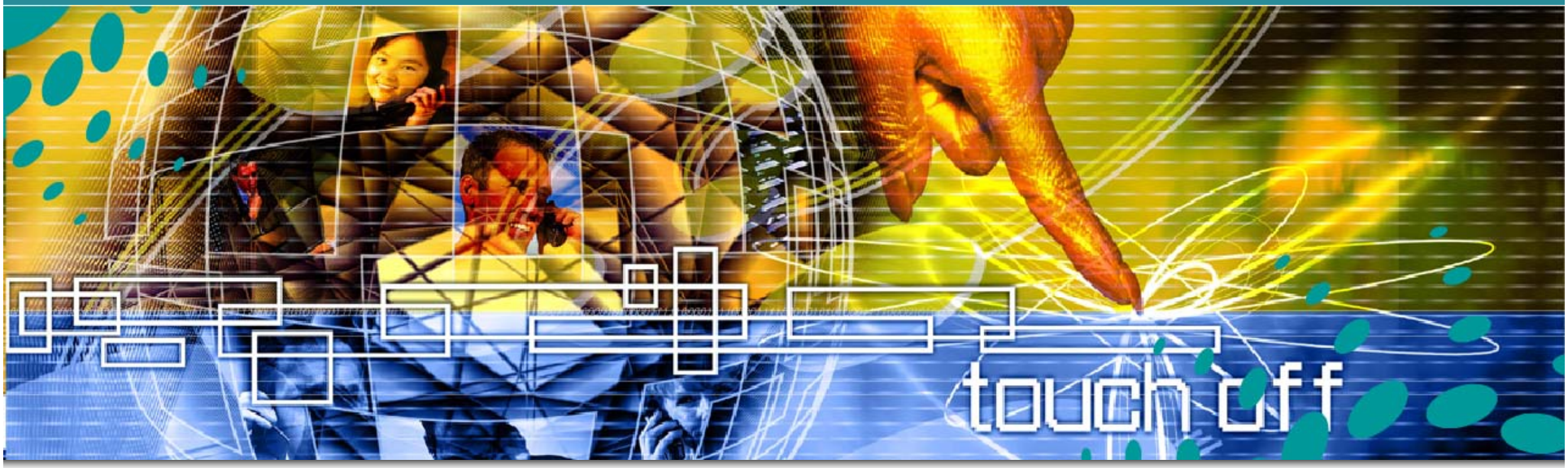
An Overview of Center for Frontiers of Subsurface Energy Security (CFSES)



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SciDAC-e

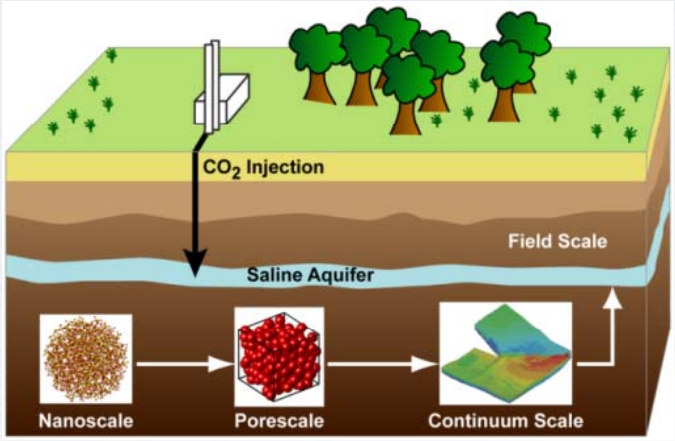
July 14, 2010

Frontiers of Subsurface Energy Security

Center for Frontiers of Subsurface Energy Security
Gary. A. Pope, Director, The University of Texas

http://www.utcfses.org/

Summary statement: Our goal is scientific understanding of subsurface physical, chemical and biological processes from the very small scale to the very large scale so that we can predict the behavior of CO_2 and other byproducts of energy production that may need to be stored in the subsurface.



RESEARCH PLAN AND DIRECTIONS

- Challenges and approaches: Integrate and expand our knowledge of subsurface phenomena across scientific disciplines using both experimental and modeling approaches to better understand and quantify behavior far from equilibrium.
- Unique aspects: The uncertainty and complexity of fluids in geologic media from the molecular scale to the basin scale.
- Outcome: Predict long term behavior of subsurface storage.

TEXAS

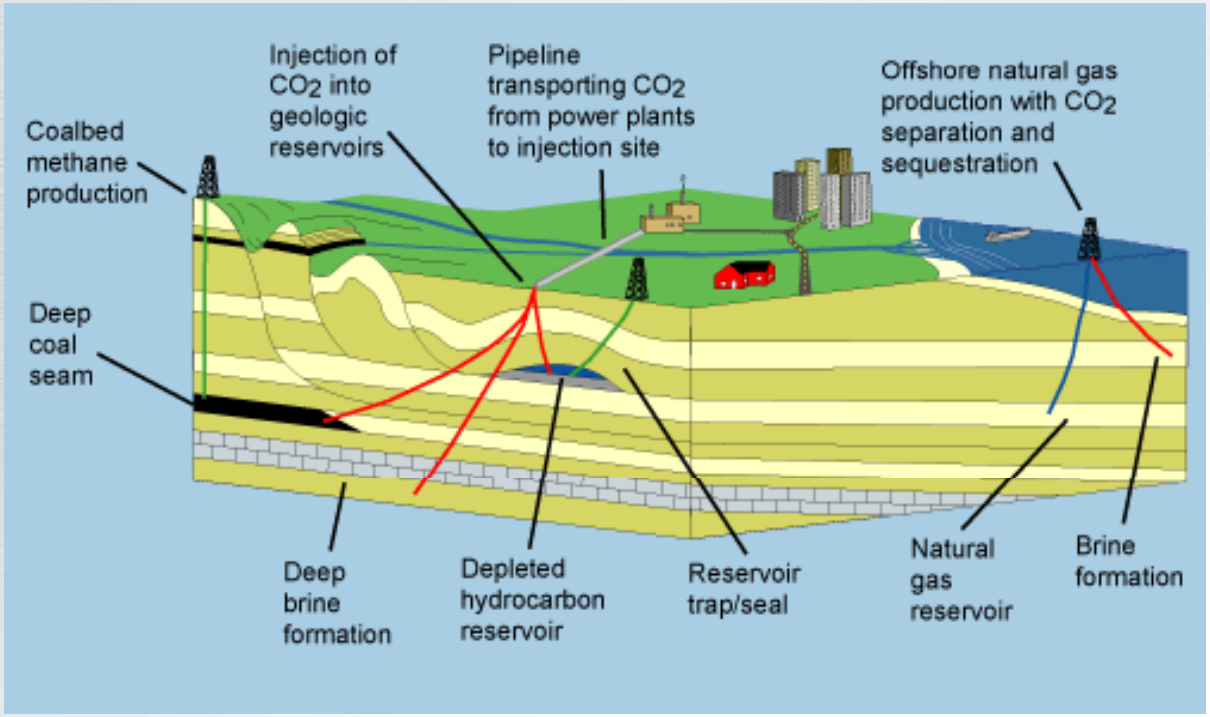
U.S. Department of ENERGY-BES

Sandia National Laboratories

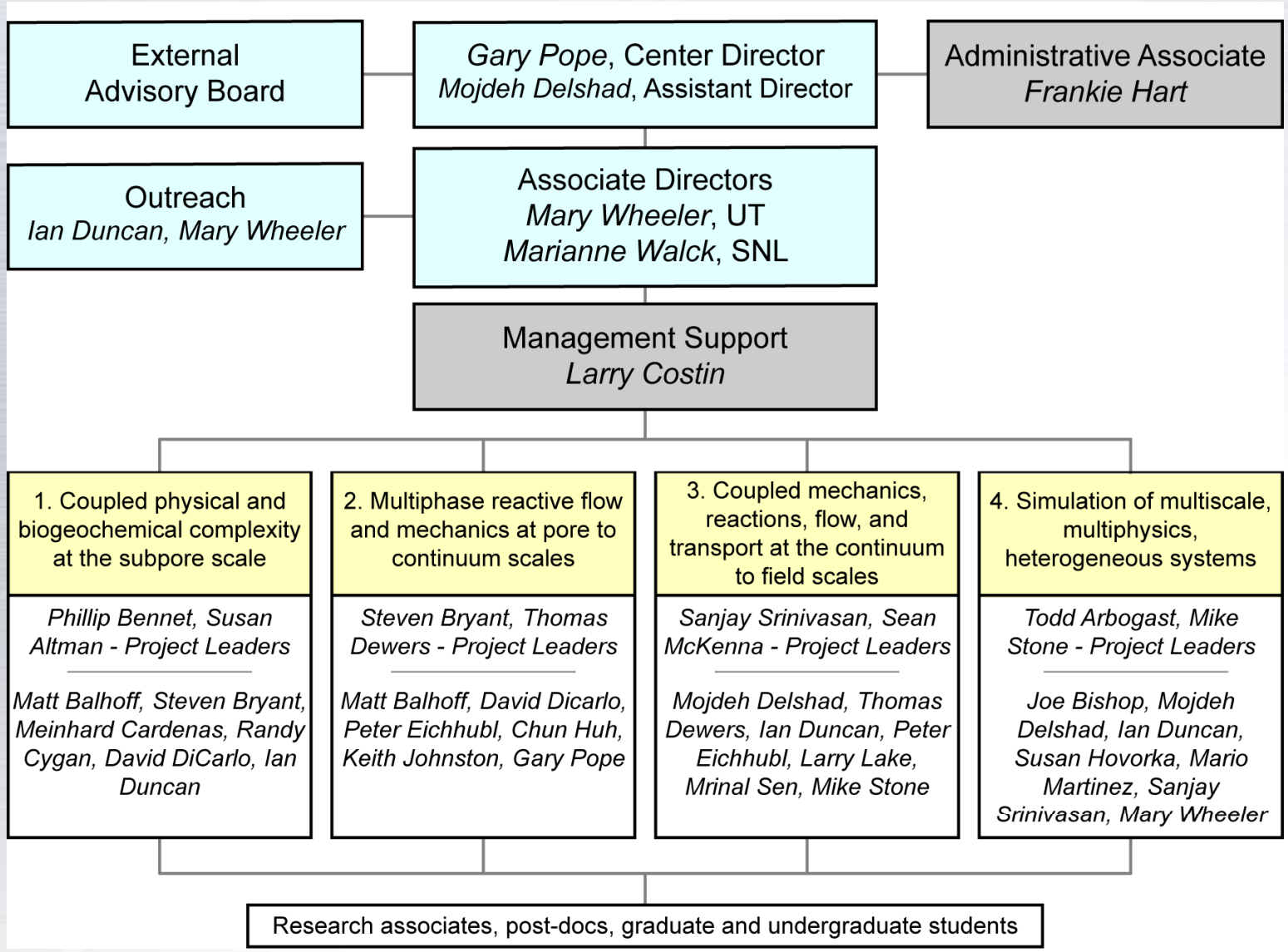
CO_2 Sequestration

Potential Sinks for CO_2 Storage:

- Deep Saline Aquifers
- Mature Oil and Gas Fields
- Deep Coal Seems



CFSES Management Structure



Highly Integrated Multidisciplinary, Multiscale, Multiprocess

Center for Frontiers of Subsurface Energy Security (CFSES)

- Multidisciplinary research goals to bridge the physical, biogeochemical, and geomechanical phenomena across multiple scales from subpore to field scale
- Interdisciplinary team of biologists, chemists, computational scientists, engineers, geologists, and mathematicians
- Integrate theory and computational methods directly into laboratory and field studies
- Address grand-challenge carbon sequestration problem

Coupled Physical and Biogeochemical Complexity at the Subpore Scale

Research Focus Area 1

Vision and Goals

- Understand CO_2/brine/geo/bio pore scale behavior
  - fully flexible CO_2 molecular dynamics simulations;
  - CO_2 and H_2O interfacial processes through MD modeling and high PT experiments;
  - pore scale CO_2+brine fluid flow
  - CO_2 – Mineral microbe reactions and transport

Challenges and Opportunities

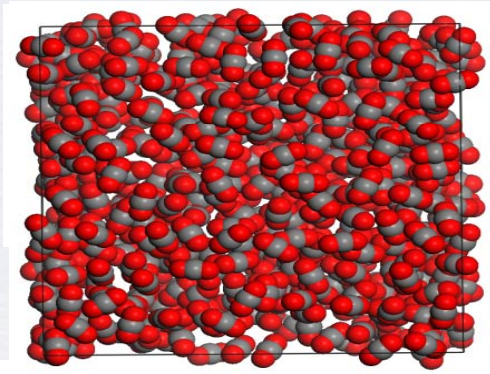
- Developing CT scanned column flow apparatus
- Deep CO_2 injection test - SECARB phase 3,
  - 180 gas samples analyzed & interpreted to characterize CO2-water-rock interactions.

Accomplishment and Highlights

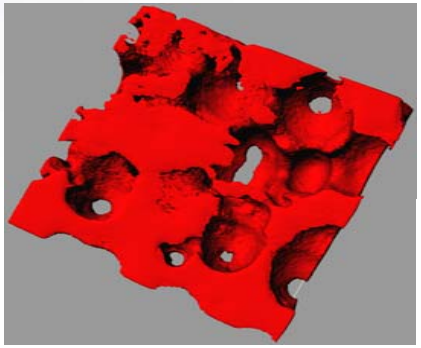
- Characterized microbial survival at high CO_2 pressures
- Tested brine/CO_2/Microbe reactor design.

Path Forward

- Experimental determination of Ca-brine/CO_2/CH_4 EOS
- Measurements of metal mobility
- Measurements of microbial survival on minerals



Molecular dynamic simulation 512 CO_2 molecules



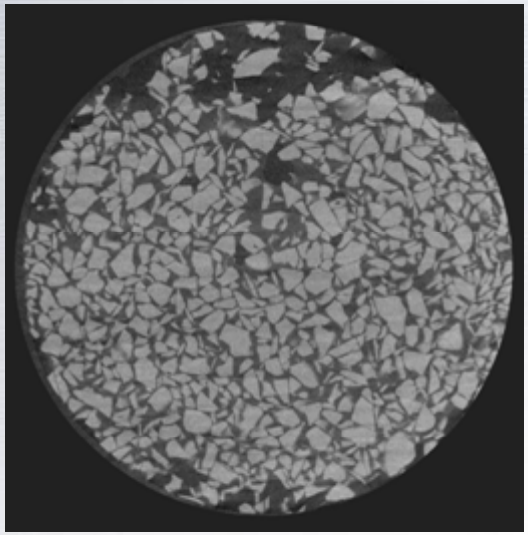
Confocal laser scanning image of pore-space

Collaborations: Framework

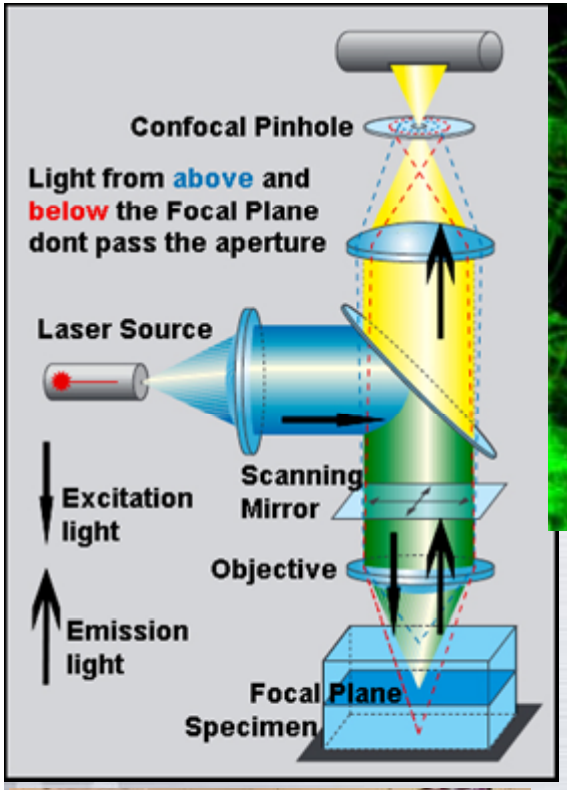
- CFSES is organized around 4 scales of observations, coordinated to achieve integration and synergy across these scales.
- Each of the focus areas work within their scope of interest, while passing out critical results to other focus areas, incorporating results, interpretations, and opportunities from others.
- This concatenation of results ensures that data from one area can be upscaled (or downscaled), and that results are validated by information or investigations at other spatial and temporal scales.
- The organizational design compels the research focus areas to interact extensively and to coordinate their activities

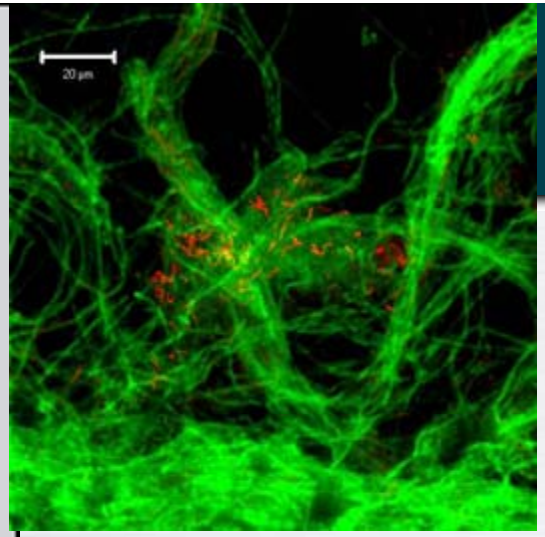
Collaborations: X-ray CT lab

- The High Resolution X-Ray CT facility at the university of Texas is a NSF multi-user laboratory facility that will be a focus of activity across scales.
- This facility, housed in the Jackson Geosciences Building, offers ready access to conduct experiments with resolutions <5μm, or object sizes >30cm



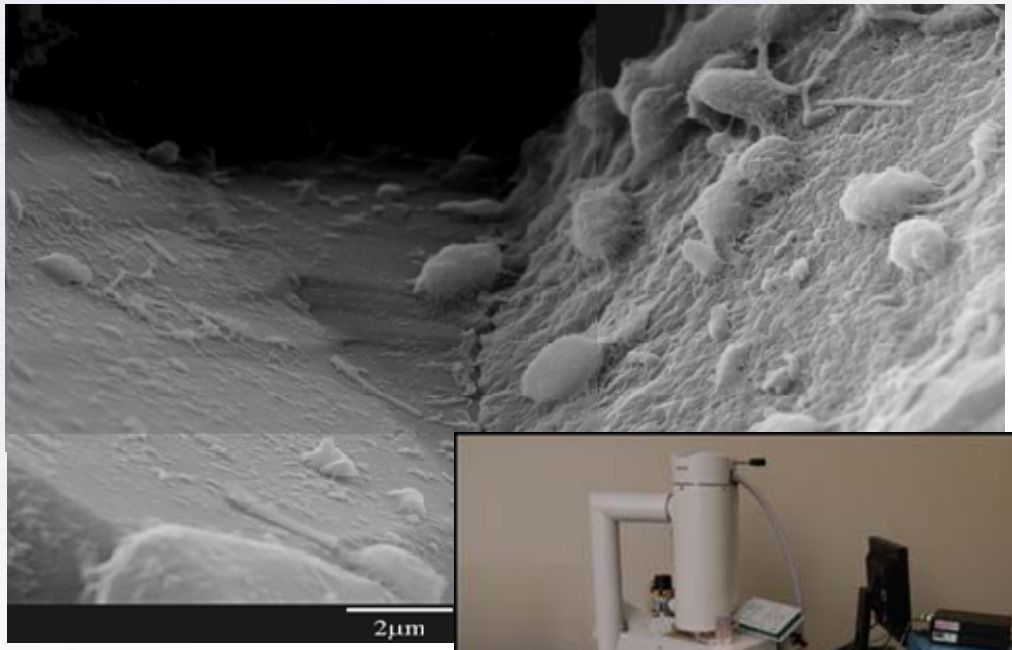
Gas, water, and quartz sand in high pressure column capable of flowing sc CO_2.



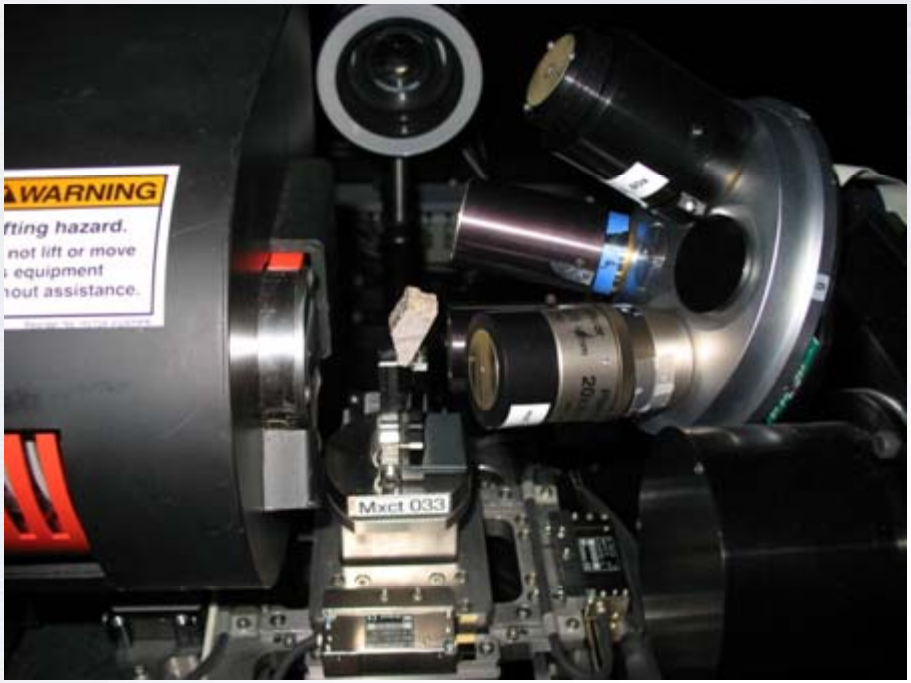


- Paired labs using model materials and organisms with shared experimental goals allow collaboration while still taking advantage of institutional strengths.

SNL Confocal imaging lab for biofilms



UT-CT Facility



- Will be used for imaging $scCO_2$/water/minerals/biofilm in static and column dynamic experiments
- XRadia MicroXCT
  - 150 kV Hamamatsu closed source; spot size to 4-7 µm
  - Cone beam data collection (up to 2048 slices)
  - Voxel size down to 0.2 µm, line pair detection to 1.5 µm
  - Successfully tested with high pressure multi-phase fluids in PEEK column

In situ observations in diamond cell

Jung-Fu Lin

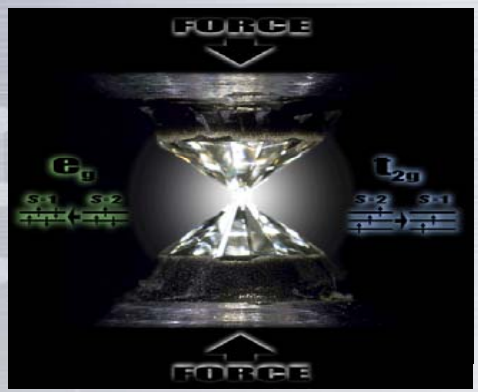
Mineral Physics

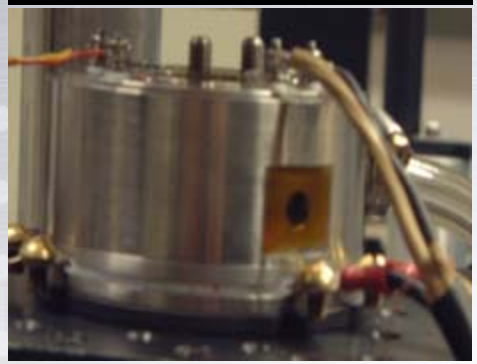
- Phase identification/transitions
- Crystal/Local structures
- Sound velocities
- Transport properties (i.e., thermal)
- Local electronic structures
- Dynamic, kinetics of reactions

High P-T Techniques

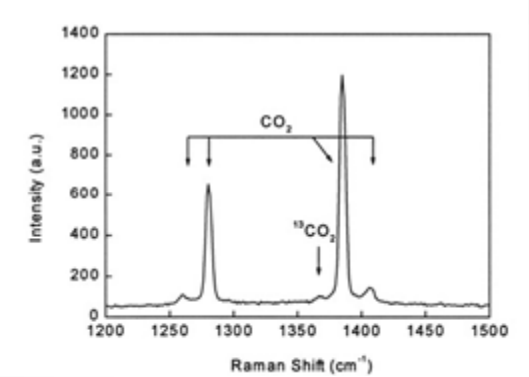
- Optical Raman/IR
- X-ray Diffraction
- Inelastic X-ray and Brillouin spectroscopies
- Time-resolved laser spectroscopy
- X-ray Raman spectroscopy
- Dynamic diamond cell with fast detectors

Hydrothermal Diamond Cell

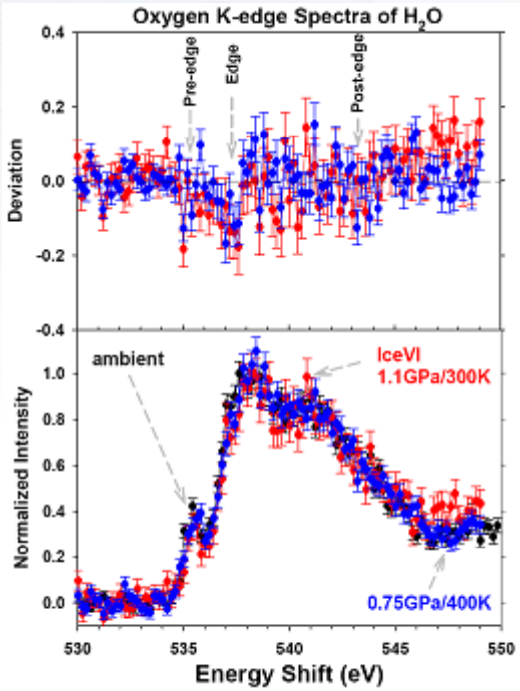




Raman System at Jackson School



Advanced Synchrotron Spectroscopies



(X-ray Raman spectra of liquid H2O)

Mechanics and Flow at the Pore-to-Continuum Scale

Research Focus Area 2

Vision and Goals

- *Characterizing perturbed natural systems*
- *Modeling across time and length scales*
- *Imaging flow and deformation*
- *Engineering of perturbed multiphase systems*

Challenges and Opportunities

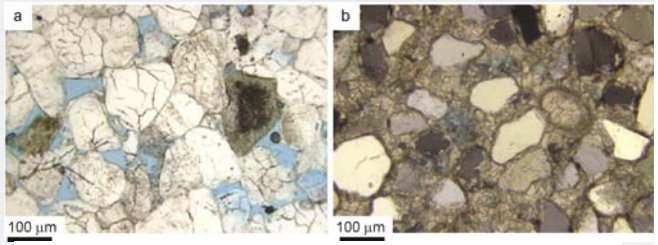
- *Upscaling and downscaling between pore and continuum multiphysics*
- *Capturing nonlinear coupling, resulting feedbacks and emergent phenomena*

Accomplishments and Highlights

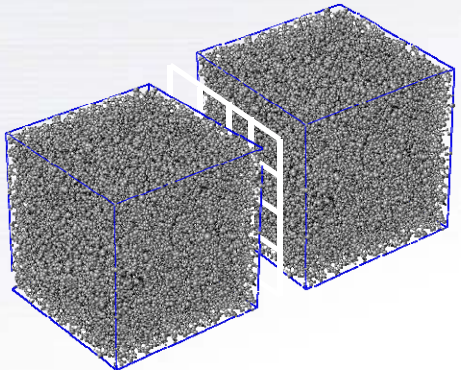
- *New imaging and flow labs*
- *Proof of concept of in situ CO2 foam generation*
- *Field investigation at Crystal Geyser, Utah*
- *Mortar method for pore-to-FEM models*

Path Forward

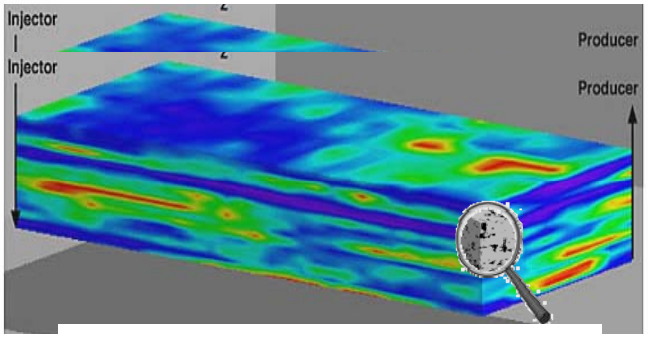
- *Testing hypotheses and assumptions about multiphase flow*
- *Integrating field, lab, and model*



Sandstone pores unaltered (a) and altered (b) by exposure to CO2



Using FEM mortars to link pore-level descriptions



Pore-to continuum upscaling

Coupled mechanics, reactions, flow & transport at the continuum to field scales

Research Focus Area 3

Vision and Goals

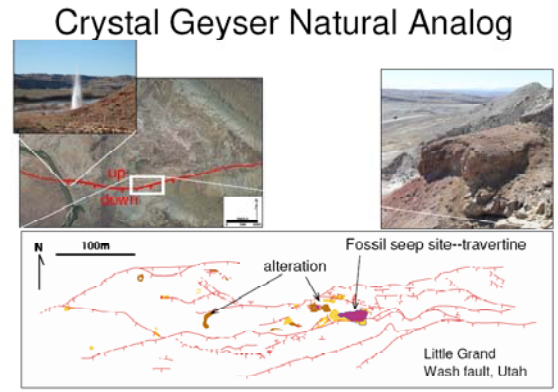
Develop scientific understanding of reactivation and seepage of fluids along faults/fractures through experimental and field scale characterization, modeling and monitoring

Challenges and Opportunities

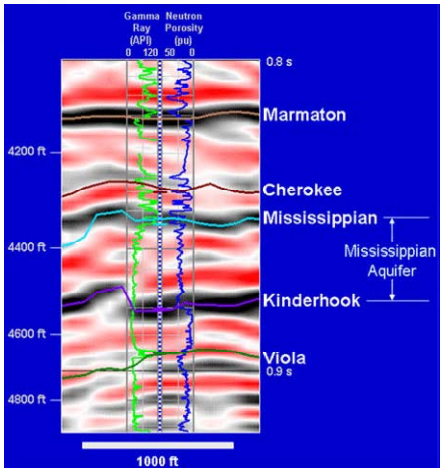
- Characterization, modeling and monitoring of reactivation and seepage of fluids along faults
- Understanding and analyzing scale up characteristics of subsurface processes
- Seismic monitoring of a sequestration field site, prior, during and post injection

Accomplishment and Highlights

- Determined CO_2 reservoir escape paths at Crystal Geyser natural analog using mineralogical analysis
- Improved reservoir characterization using seismic for the CO_2 sequestration project at Dickman, Kansas
- Mathematical/statistical scale-up analysis of flow processes
- **Path Forward**
- Analyze pressure and injection data at Cranfield site to determine signature of faults on the data collected
- Develop faster cellular automata model to describe episodic behavior of faults subject to high-pressure fluid source.



Dickman site, KS – US DOE funded CO2 sequestration project



Simulation of Multiscale, Multiphysics, Heterogeneous Systems

Research Focus Area 4

Vision and Goals

- Synthesize and build upon first 3 Focus Areas
- Develop cutting-edge couplings across scales
- Model and simulate the subsurface to make long-term, reservoir scale predictions

Challenges and Opportunities

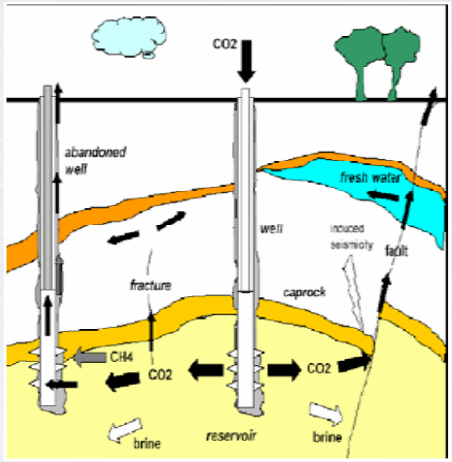
- What models are needed to assess CO_2 fate?
- How do fluids flow in damaged cap rocks?
- How can we be computationally efficient?

Accomplishment and Highlights

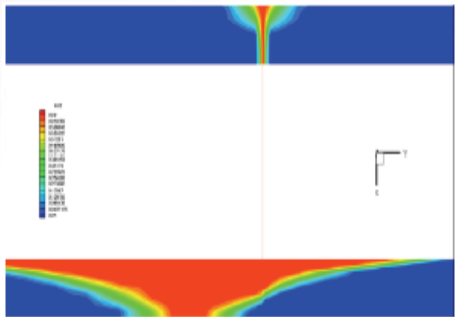
- Preliminary simulations of field pilot test data
- Multiscale and general gridding methods
- Simulation of flow in pervasive fractures

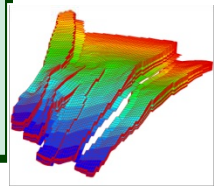
Path Forward

- Work with other Tasks for needed models
- Create novel physics-based simulation tools



Modeling fluid flow and geomechanics with fractures





CO_2 leakage through an abandoned well

Some Specific Objectives of Focus Area 4

- Models and Numerics
  - **Modeling multiphase compositional flow in realistic geometries.**
  - **Assessment of numerical accuracy via adaptive error estimators.**
  - **Enhance phase behavior and physical property models.**
  - **Multiscale modeling of medium heterogeneities.**
  - **Modeling geomechanical effects on the medium, including fractures.**
  - **Couplings and Solvers**
  - **Coupling of geochemical, geomechanical, and geobiological multiscale processes with flow and transport.**
  - **Implementation of efficient and accurate parallel multiscale and multiphysics solvers and time-stepping.**
- Field studies of CO2 demonstration sites that include parameter estimation (V&V) and uncertainty quantification.

Assumptions and Governing Equations for a Gas Flooding Process

Applying Inspectional Analysis

Assumptions:
-2 dimensional vertical cross section
-3 three components (Solvent, light-oil component, heavy-oil component)
-3 phases (Oil, Gas, water)
-No chemical reactions
-No adsorption

Total number of unknowns: 21
-9 compositions $N_p \times N_c$
-3 saturations N_p
-3 phase pressures N_p
-6 Darcy velocities $N_p \times N_D$

Total number of Equations: 21
-3 conservation equations N_c
-6 phase equilibrium equations $N_c \times (N_p - 1)$
-2 capillary pressure equations $N_p - 1$
-6 Darcy's law equations $N_p \times N_D$
-1 saturations sum to 1 1
-3 mole fractions sum to 1 N_p

Conservation Equations

$$\frac{\partial}{\partial t}\phi\sum_{j=1}^{n_p} x_{ij}\rho_j S_j + \nabla\cdot\sum_{j=1}^{n_p} x_{ij}\rho_j \vec{u}_j - \nabla\cdot\phi\sum_{j=1}^{n_p}\overline{\overline{K}}_{ij}\cdot\nabla\rho_j x_{ij} = 0$$

Darcy's Law Equations

$$\vec{u}_j = -\frac{kk_{rj}}{\mu_j}(\nabla P_j + \rho_j \vec{g})$$

Capillary Pressure Equations

$$P_j - P_k = P_{ckj} = j(S)\sigma_{kj}\sqrt{\frac{\phi}{k}}$$

Phase Equilibrium Equations

$$P = \frac{RT}{V-b} - \frac{a(T)}{(V+c)(V+2c+b)+(b+c)(V-b)}$$

Saturations and

$$\sum_{i=1}^{n_c} x_{ij} = 1 \qquad j = 1, n_p \qquad \sum_{j=1}^{n_p} S_j = 1$$

41 Parameters and 27 Dependent Variables

Peng-Robinson Equation of State

$$P = \frac{RT}{\bar{v} - b} - \frac{a}{\bar{v}(\bar{v} + b) + b(\bar{v} - b)}$$

$$a = 0.45724 \frac{R^2 T_c^2}{P_c} \alpha(T) \qquad b = 0.07780 \frac{RT_c}{P_c}$$

$$\sqrt{\alpha} = 1 + f_w \left(1 - \sqrt{\frac{T}{T_c}} \right)$$

$$f_w = \begin{cases} 0.37464 + 1.54226\omega - 0.26992\omega^2 & \omega < 0.49 \\ 0.379640 + 1.485030\,\omega - 0.164423\,\omega^2 + 0.016666\,\omega^3 & \omega \geq 0.49 \end{cases}$$

Peng-Robinson Equation of State

$$a_i = \frac{0.45724 R^2 T_{c_i}^{\ 2}}{P_{c_i}} [1 + f_{w_i}(1 - \sqrt{T_{r_i}})]^2 \qquad b_i = 0.07780 \frac{RT_{ci}}{P_{ci}}$$

$$a_{m,j} = \sum_{i=1}^{n_c} \sum_{k=1}^{n_c} x_{ij}\, x_{kj} \sqrt{(a_i a_k)}(1 - \delta_{ik}) \qquad b_{m,j} = \sum_{i=1}^{n_c} x_{ij} b_i$$

$$Z_j = \frac{P \bar{v}_j}{RT} \qquad A_j = \frac{a_{m,j} P}{(RT)^2} \qquad B_j = \frac{b_{m,j} P}{RT}$$

$$Z_j^3 + (B_j - 1) Z_j^2 + (A_j - 3B_j^2 - 2B_j) Z_j + (-A_j B_j + B_j^2 + B_j^3) = 0$$

Fugacity Coefficients for Peng-Robinson EOS

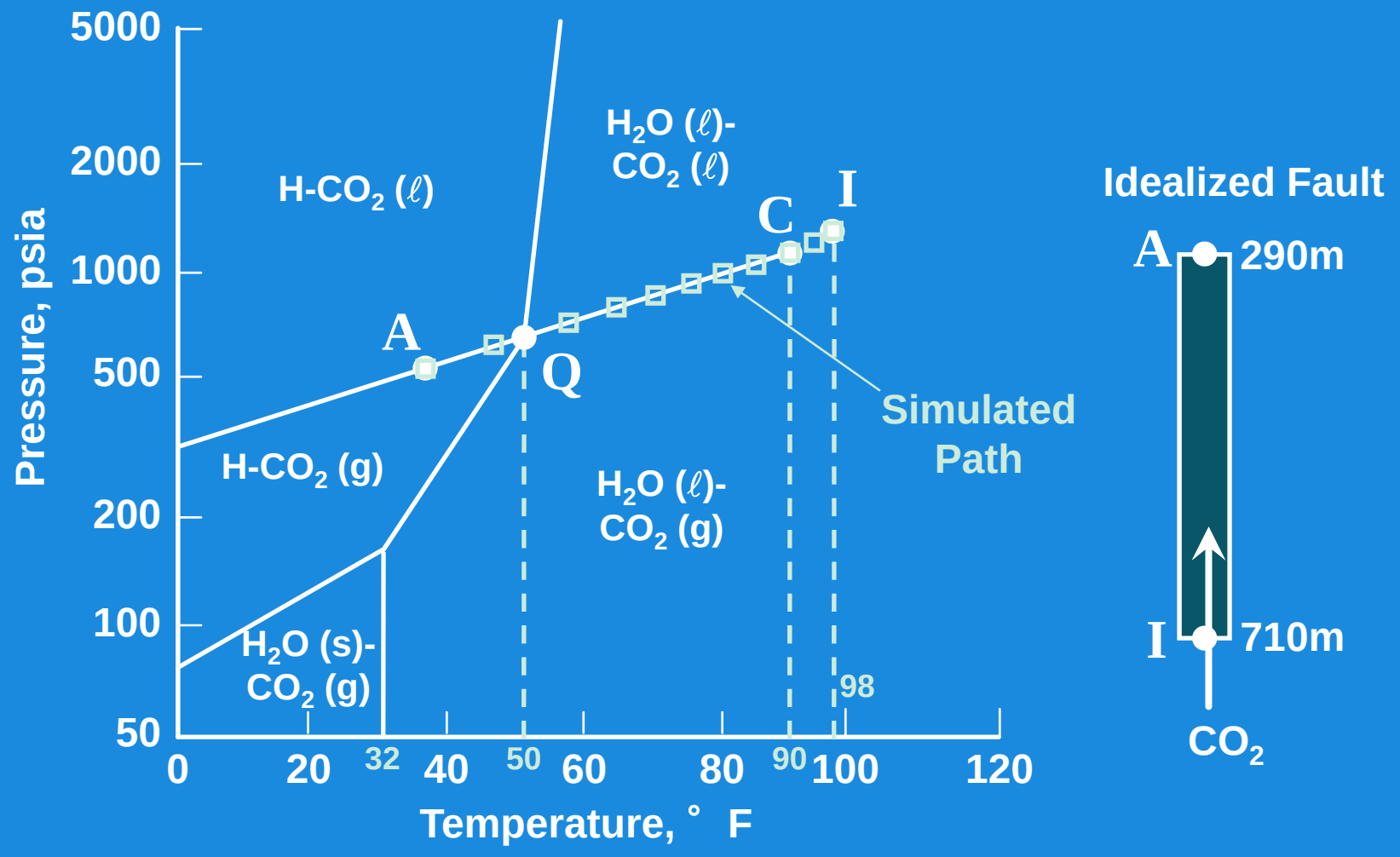
$$Ln\varphi_{ij} = \frac{b_i}{b_m}\left(Z_j - 1\right) - Ln\left(Z_j - B_j\right) - \frac{A_j}{2\sqrt{2}B_j}\left(\frac{2}{a_j}\sum_{m=1}^{n_c} x_{mj}a_{im} - \frac{b_i}{b_m}\right) Ln\left[\frac{Z_j + \left(1+\sqrt{2}\right)B_j}{Z_j + \left(1-\sqrt{2}\right)B_j}\right]$$

$$f_{ij} = \varphi_{ij} x_{ij} P$$

$$g_j = \frac{G_j}{RT} = \sum_{i=1}^{N_c} n_{ij} Lnf_{ij}$$

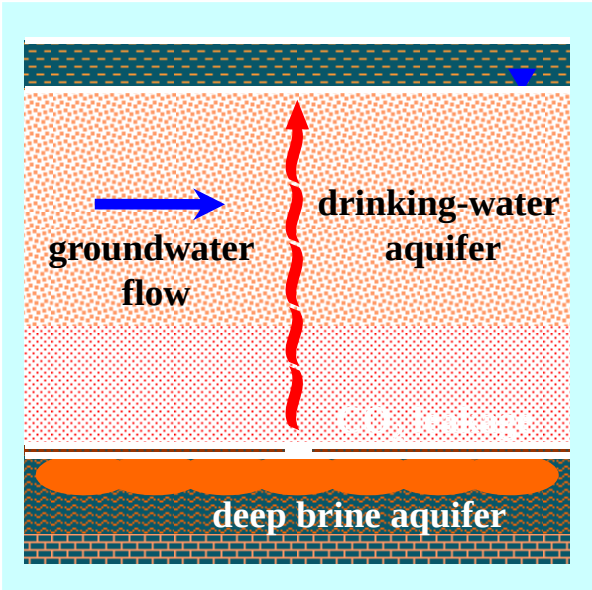
$$g_t = \sum_{j=1}^{N_P} g_j$$

Phase Diagram for H_2O-CO_2 Mixture



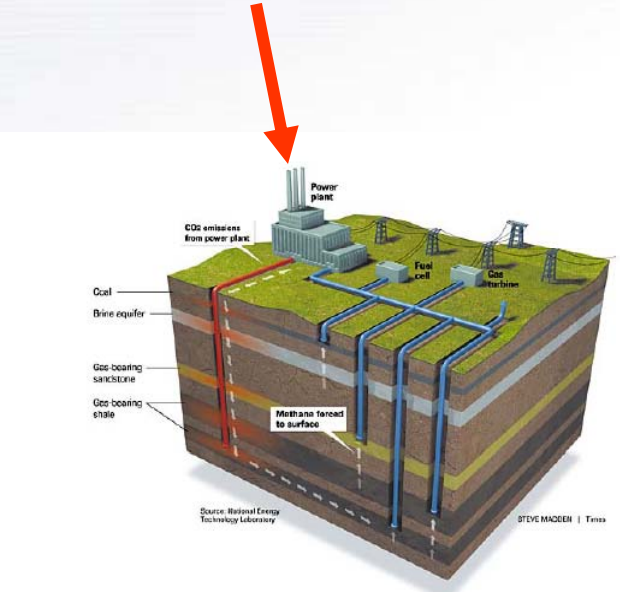
Key Issues in Storage

- What is the likelihood and magnitude of CO_2 leakage and what are the environmental impacts?
- How effective are different CO_2 trapping mechanisms?
- What physical, geochemical, and geomechanical processes are important for the next few centuries and how these processes impact the storage efficacy and security?
- What are the necessary models and modeling capabilities to assess the fate of injected CO_2?
- What are the computational needs and capabilities to address these issues?
- How these tools can be made useful and accessible to regulators and industry?

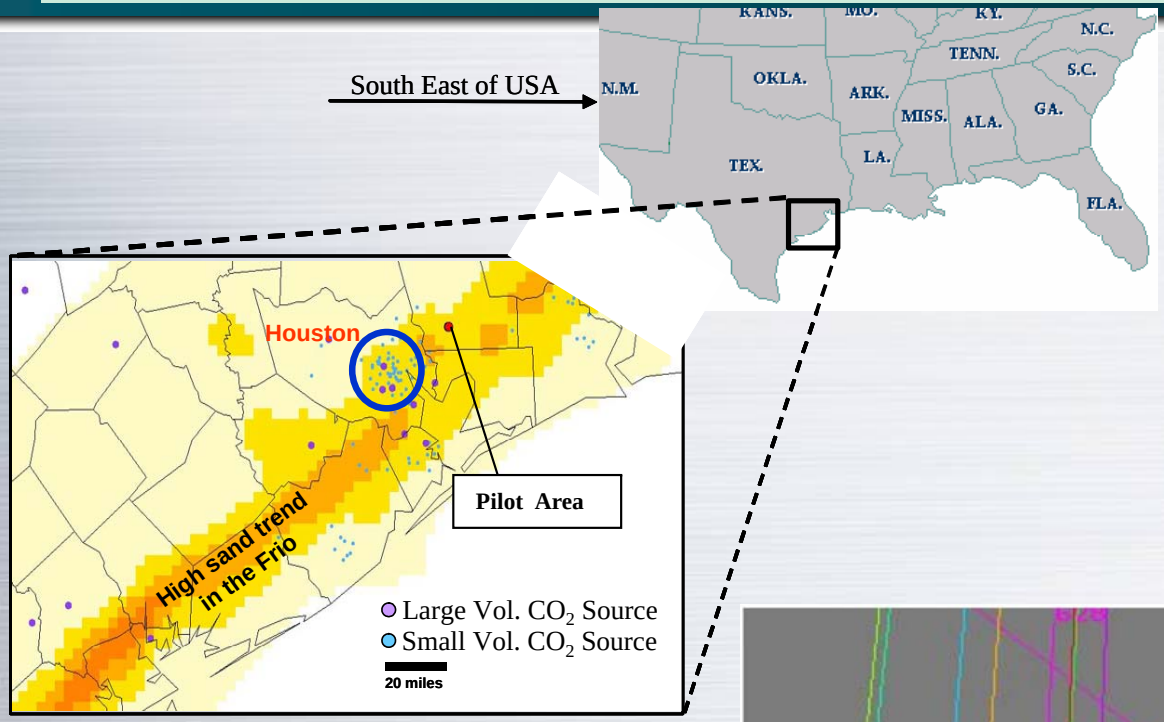


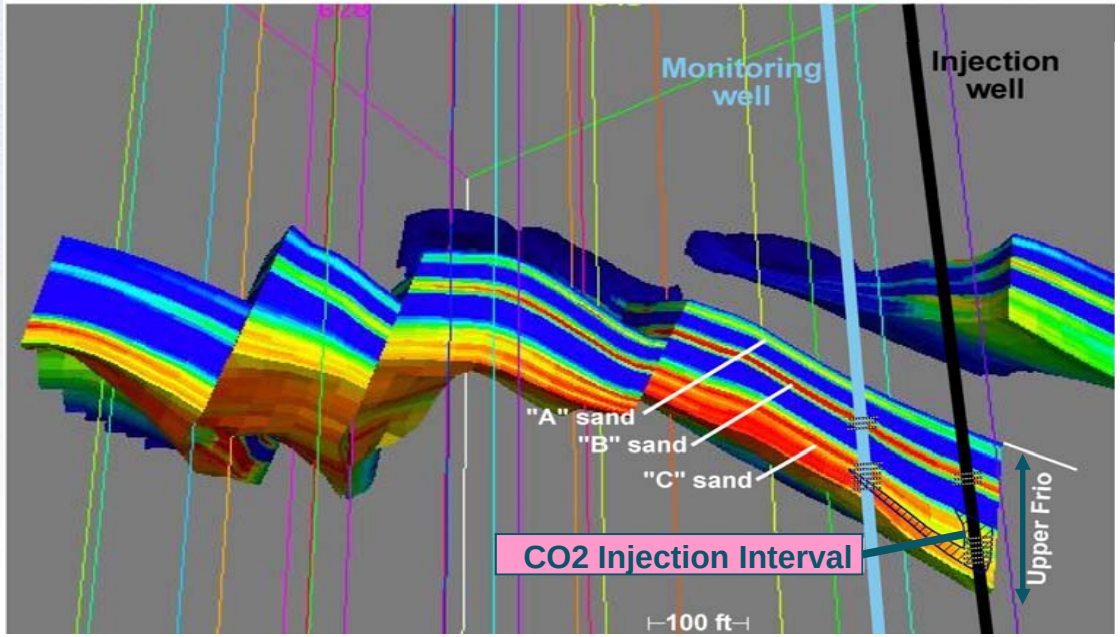
CO_2 Sequestration Modeling Approach

- **Numerical simulation**
  - ✓ Characterization (fault, fractures)
  - ✓ Appropriate gridding
  - ✓ Compositional EOS
  - ✓ Parallel computing capability
- **Key processes**
  - ✓ CO_2/brine mass transfer
  - ✓ Multiphase flow
    - ✓ During injection *(pressure driven)*
    - ✓ After injection *(gravity driven)*
  - ✓ Geochemical reactions
  - ✓ Geomechanical modeling

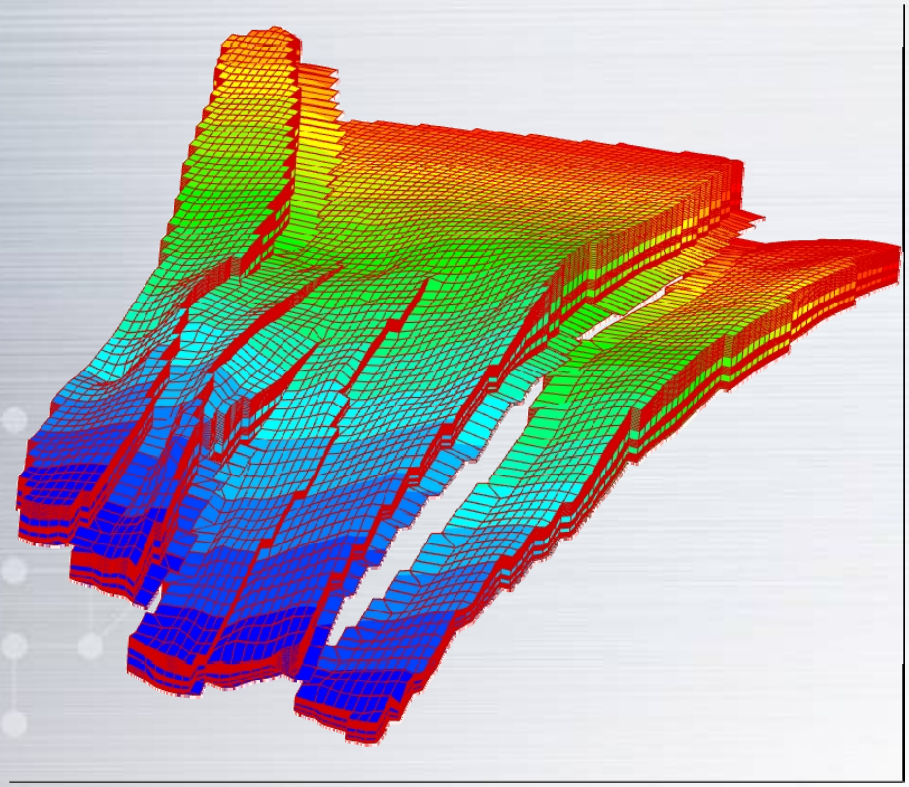


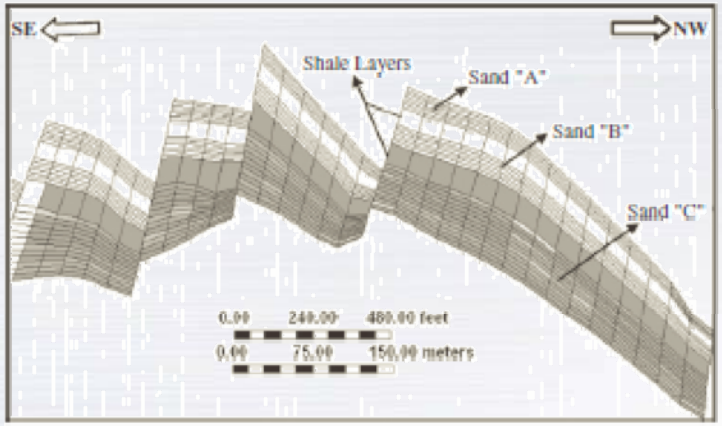
Frio CO2 Sequestration Pilot

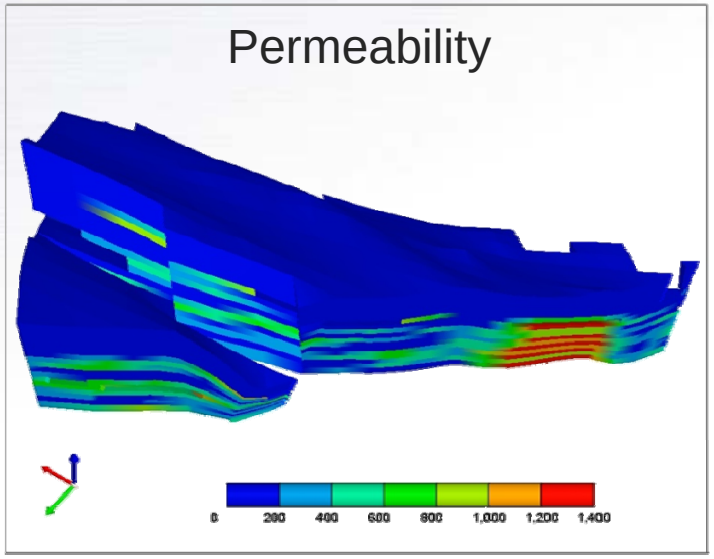




Corner Point Grid for Frio Pilot Test



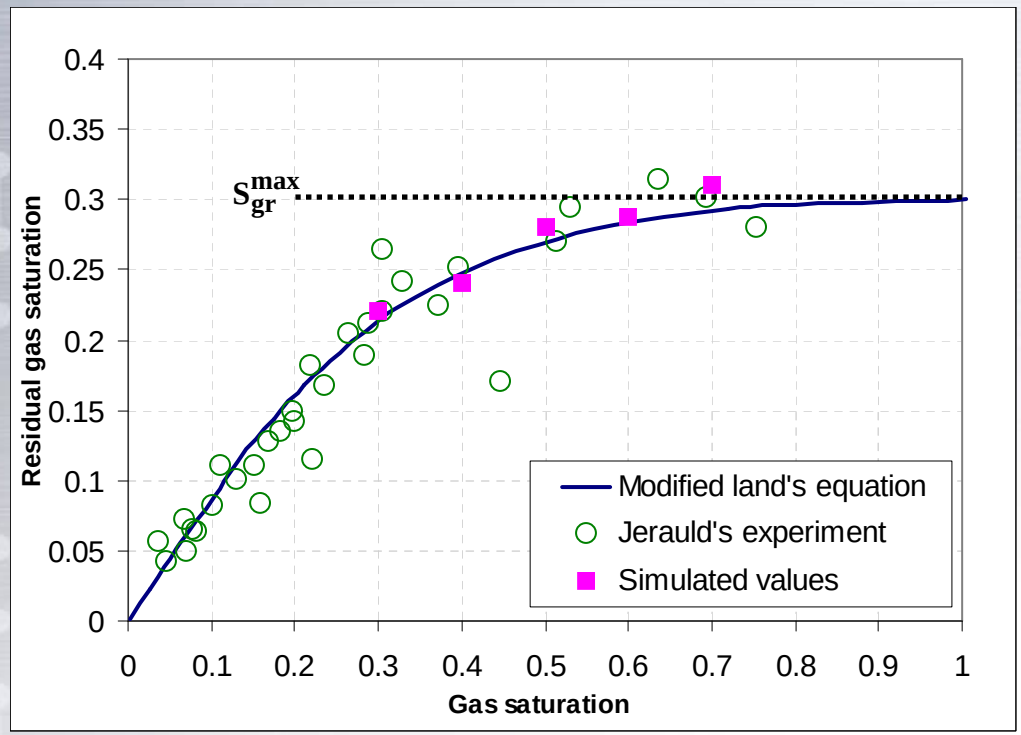




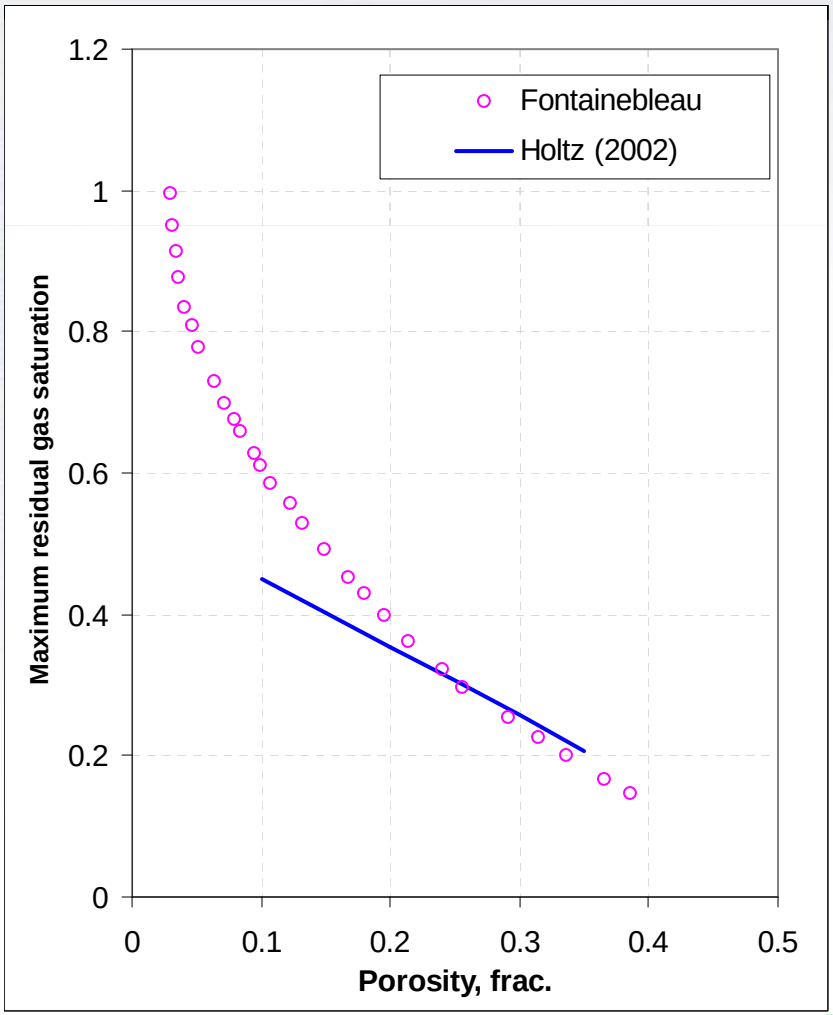
Hysteresis Model

- **Modified Land's Equation:**

$$\frac{1}{S_{gr}^{\max}} - \frac{1}{S_{g}^{\max}} = \frac{1}{S_{grh}} - \frac{1}{S_{gh}}$$



Correlation between maximum residual gas saturation, S_{gr}^{max}, and porosity

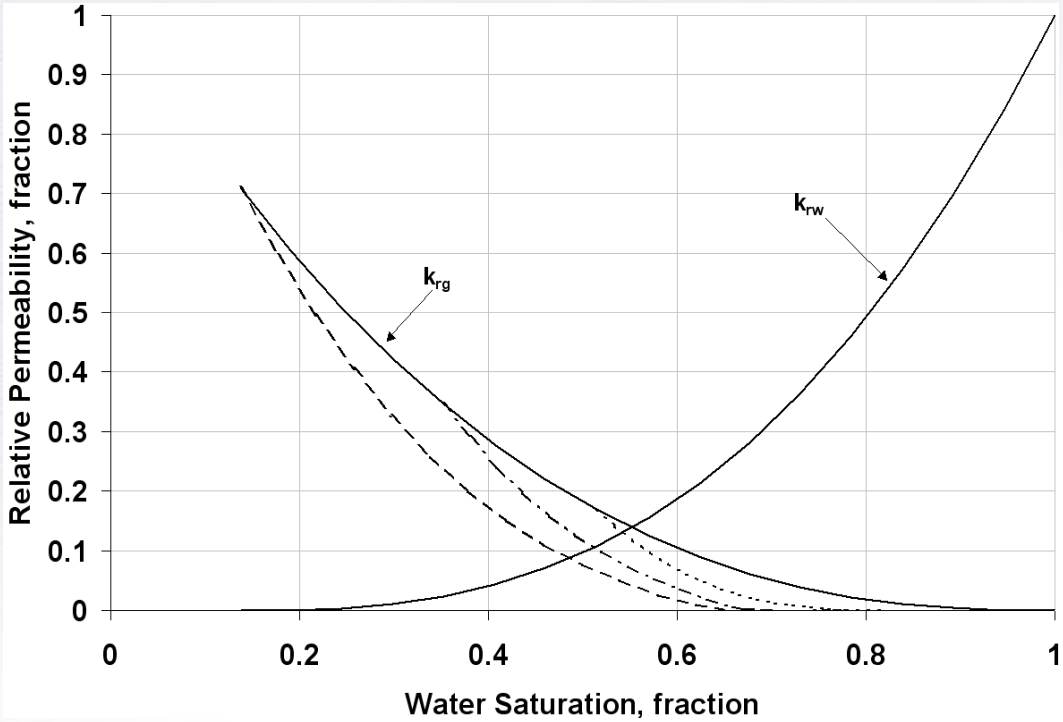


Hysteresis in Gas Relative Permeability

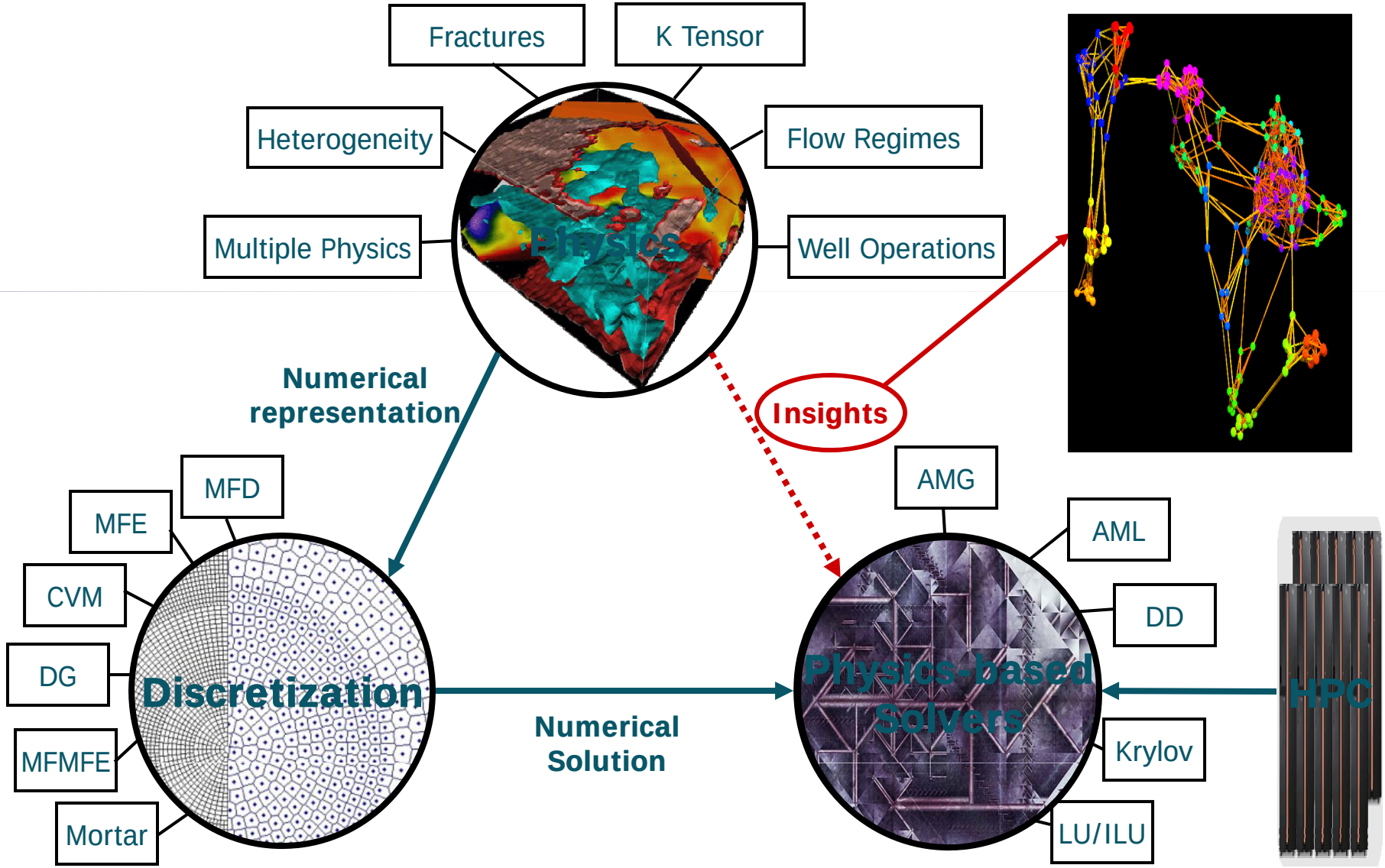
- **Jerauld's (1996) Gas Relative Permeability Model**

$$k_{rg} = \frac{(1+C_{g2})\left(\dfrac{S_g(\text{shifted}) - S_{gr}}{1-S_{gr}}\right)^{Cg1}}{1+C_{g2}\left(\dfrac{S_g(\text{shifted}) - S_{gr}}{1-S_{gr}}\right)^{C_{g1}(1+1/C_{g2})}}$$

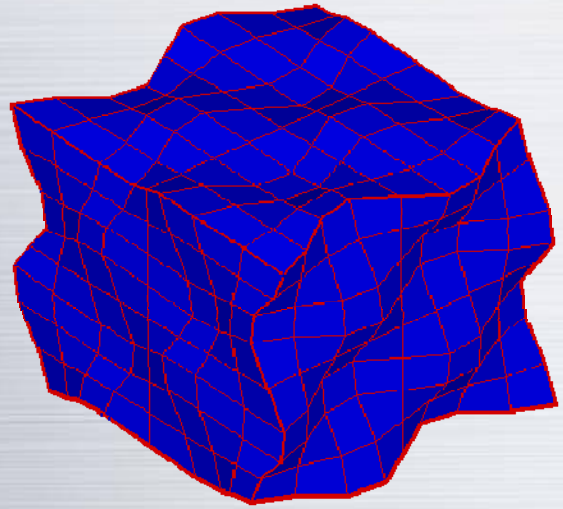
$$S_g(\text{shifted}) = S_{gr} + \frac{(S_g - S_{grh})(S_{gh} - S_{gr})}{(S_{gh} - S_{grh})}$$

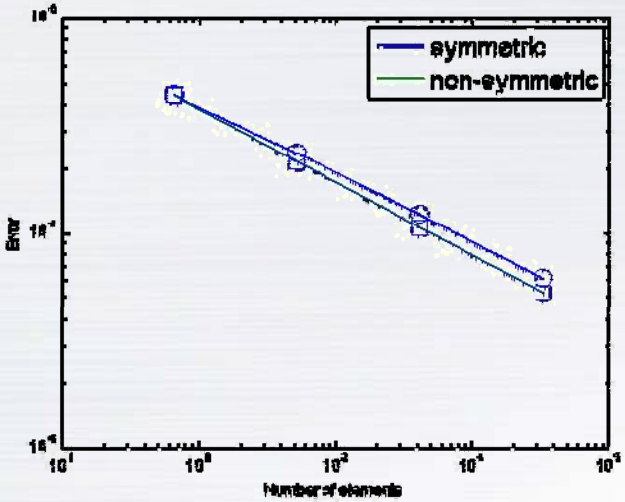


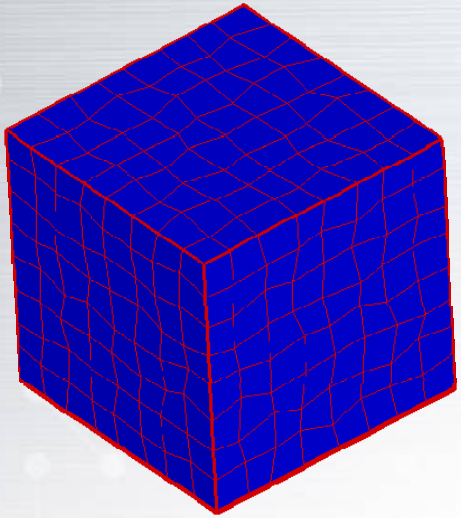
Physics Based Solvers

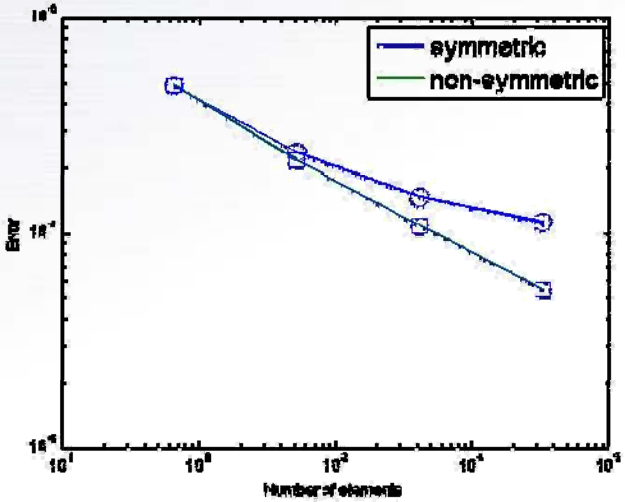


Convergence Test for MFMFE on General Hexahedra

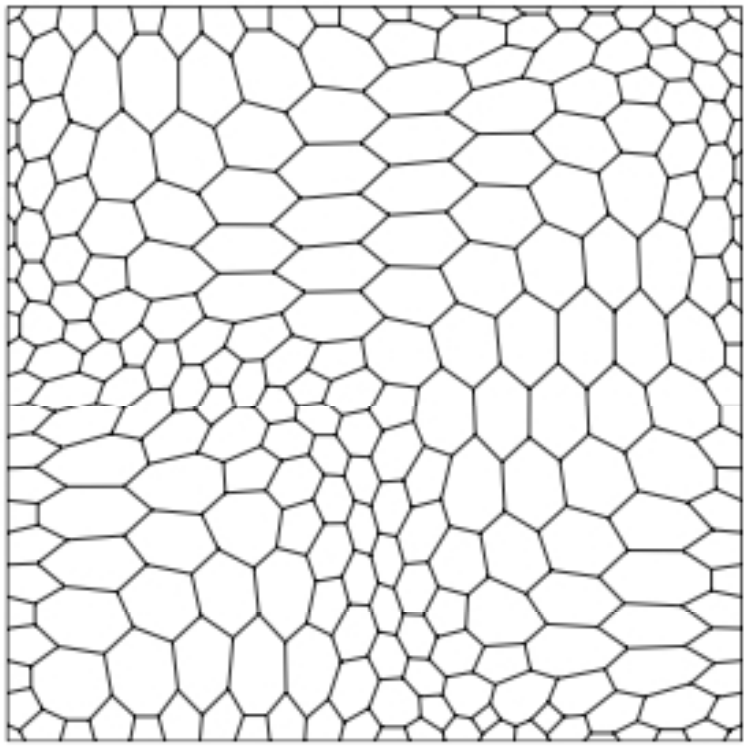


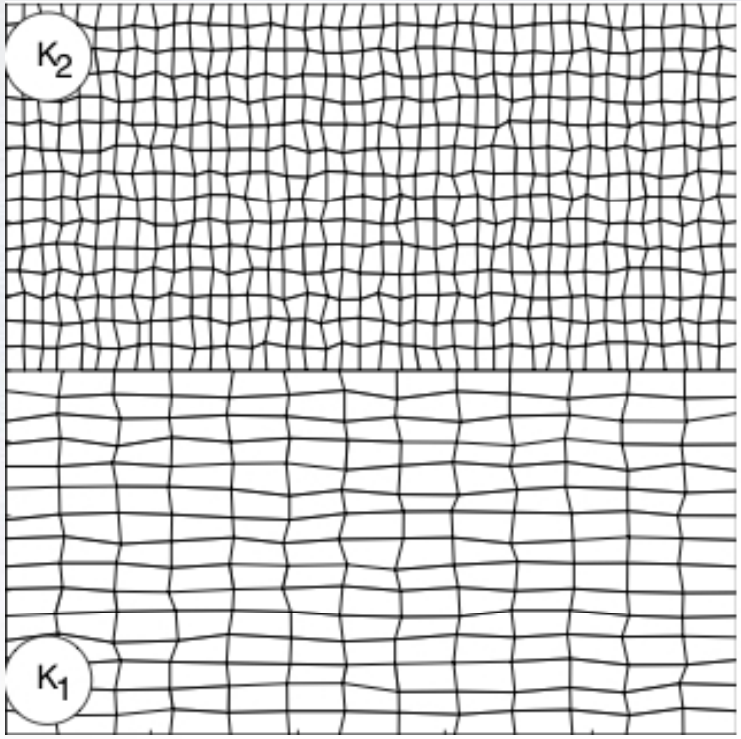






Mimetic Finite Difference Method on Polygons





Numerical Simulations of Geological Storage of Supercritical CO_2 in Deep Saline Aquifers

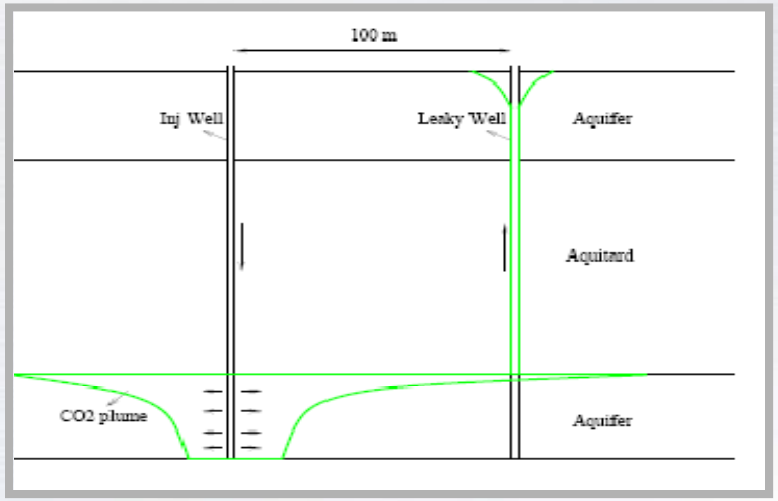
- CO2 sequestration simulation with IPARS
  - ✓ Injection strategy on sequestration performance.
  - ✓ Geological trapping mechanisms, permanent trapping.
  - ✓ Solver and grid efficiency for IPARS.

- CO2 phase behavoir and petrophysical process
  - ✓ Equation of State plays a role in modeling the CO2.
  - ✓ Comparison of CO2/water phase behavior model with measured data.
  - ✓ Model CO2 solubility in water as a function of salinity.
  - ✓ The effect of CO2 phase transition on petrophysical properties.
  - ✓ CO2 dissolution into the formation brine is affected by both P and T, as well as salinity.

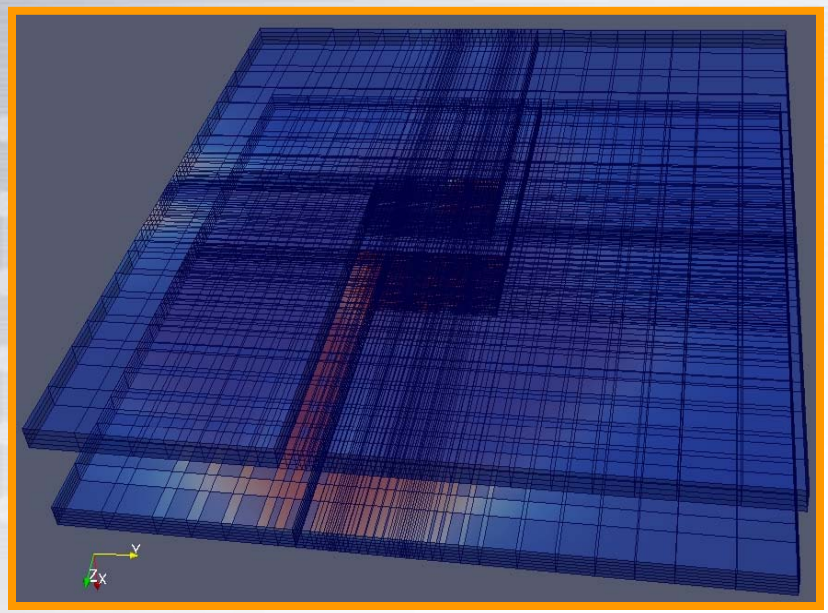
- Relative permeability hysteresis and interfacial tension
  - ✓ The impact of interfacial tension and pressure gradient under typical CO2 injection conditions on relative permeability and capillary pressure.
  - ✓ Critical review of existing hysteresis models of relative permeability and capillary pressure and comparison with published laboratory data.
  - ✓ Implementation of a hysteretic relative permeability model in IPARS.

Enhanced Velocity Method on Locally Refined Grids for CO_2 leakage Problem

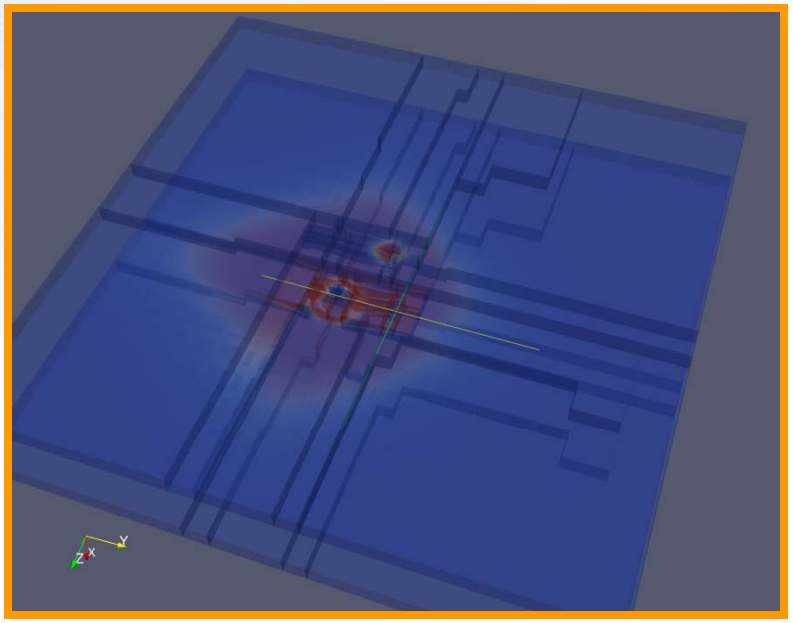
- Grid: 5 blocks 40K elements. 11x35x12, 11x37x12, 11x9x24,11x7x24,20x40x31
- Non-matching grid
- Constant pressure Dirichlet BC
- EOS, CO_2 immiscible in brine
- 24 processors



5-block non-matching grid (fine around wells)

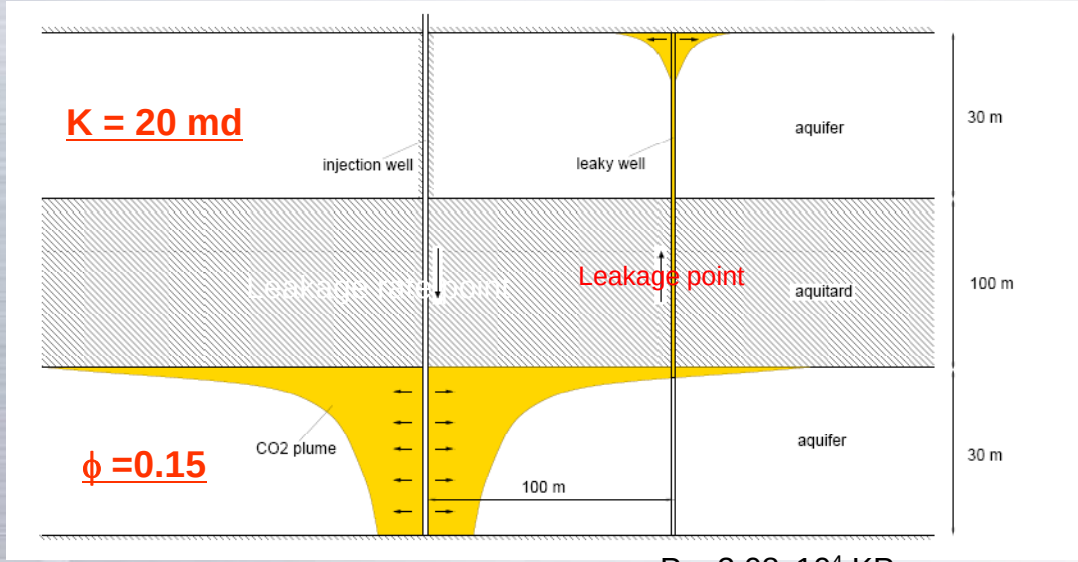


Processor distribution (dense near wells)



Simulation of CO2 Benchmark Problems

CO_2 Leakage Benchmark Problem



P = 3.08×10^4 KPa

Objective

Quantification of leakage rate in deep aquifer @2840-3000 m

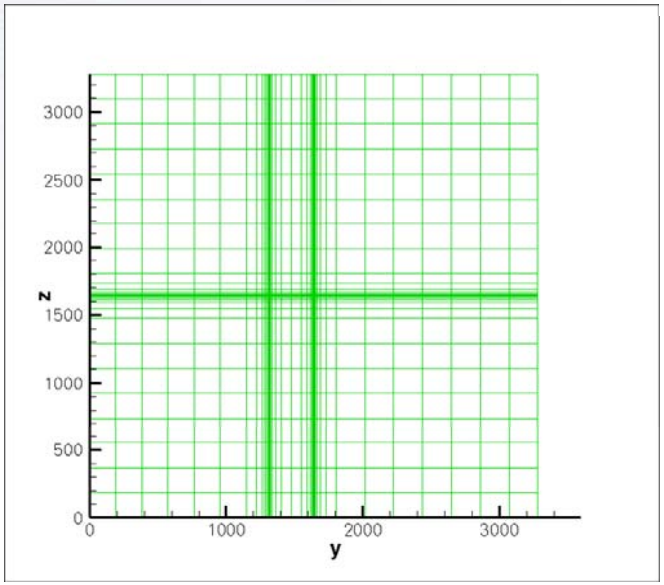
Output

1- Leakage rate = %CO_2 mass flux/injection rate

2- CO2 saturation at 1000 days

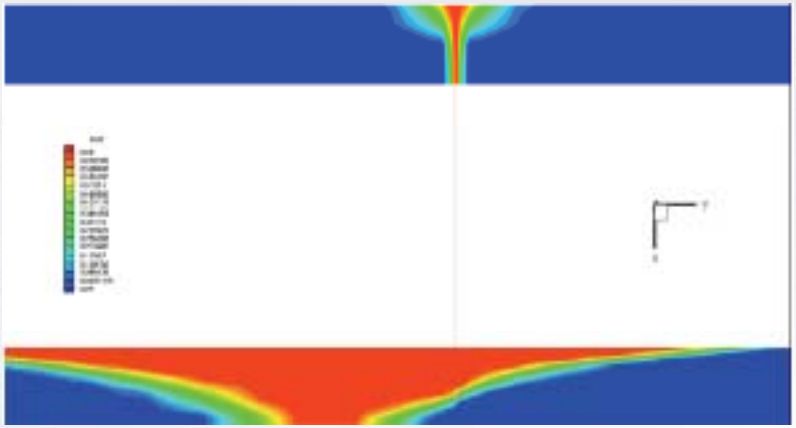
- Grid: several configurations
- Fine grid near wells
- Constant pressure Boundary condition
- Compositional model
- Parallel simulation (up to 256 processors)

Mesh



Simulation results with IPARS for two cases

CO_2 leakage through abandoned well



CO_2 saturation profile for leaky well

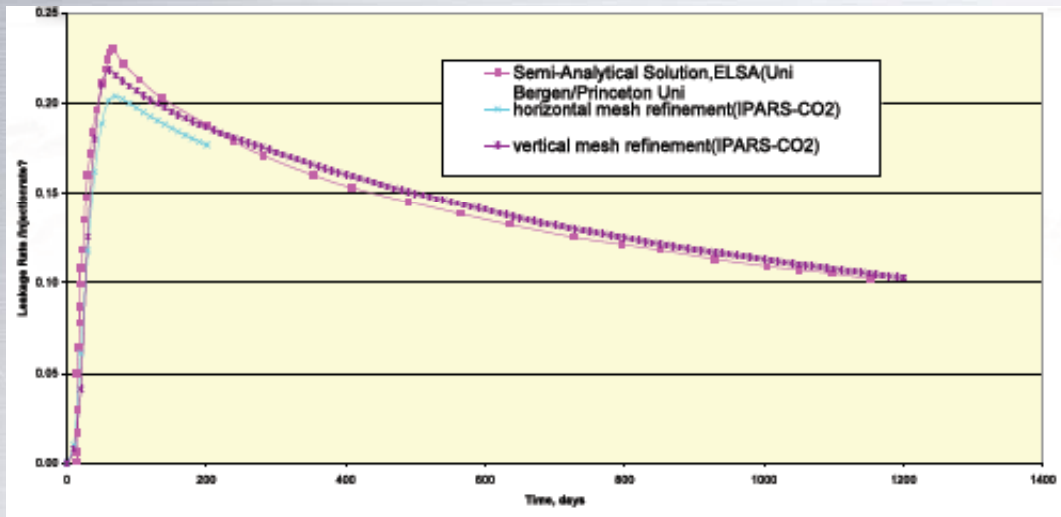
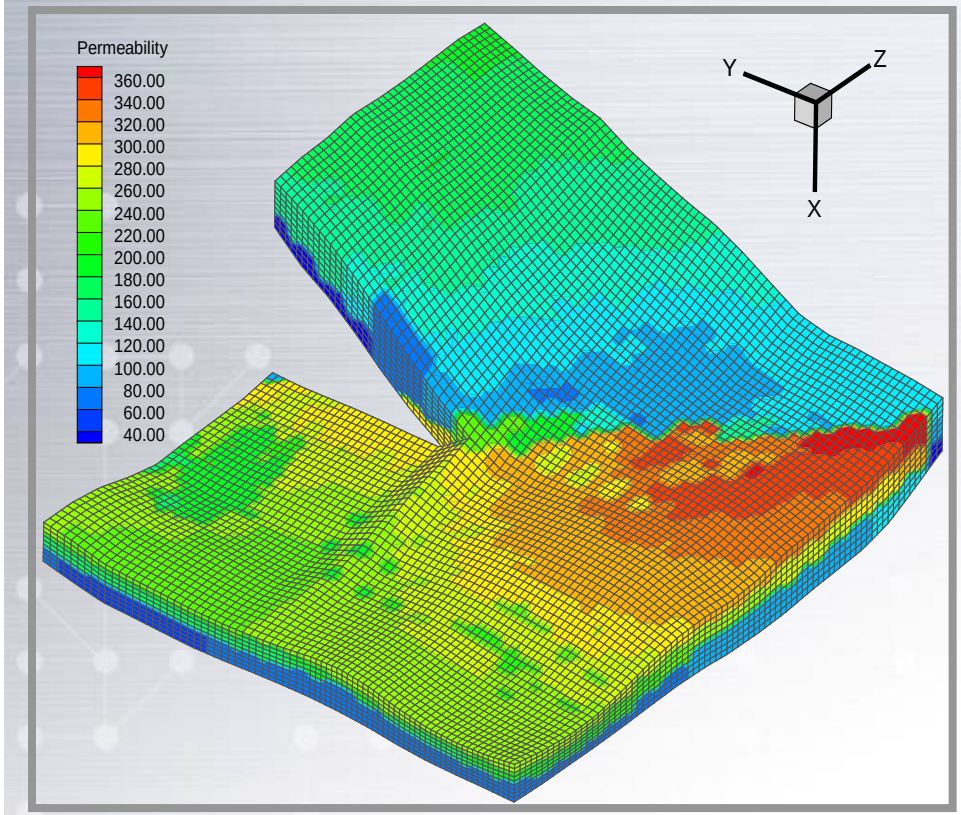


Fig. 3 CO_2 distribution over time

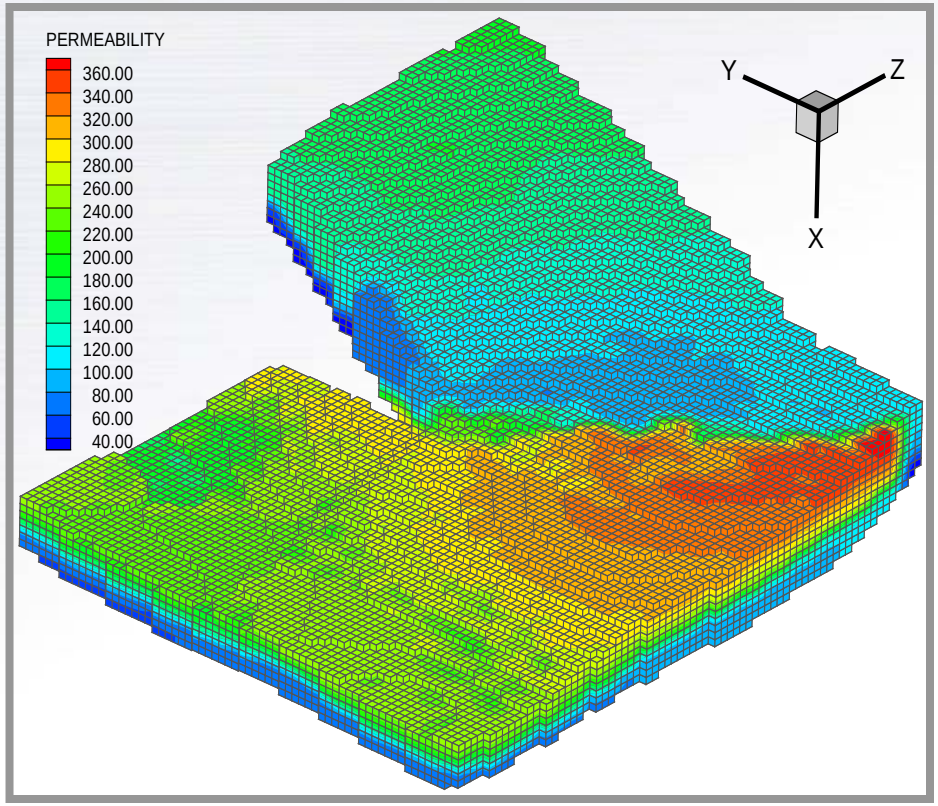
Benchmark Problem 3: Permeability

- Stair stepped approximation on a 50x100x100 grid (~75,000 active elements) used to derive approximate geometry and suitably interpolate properties.

True permeability field



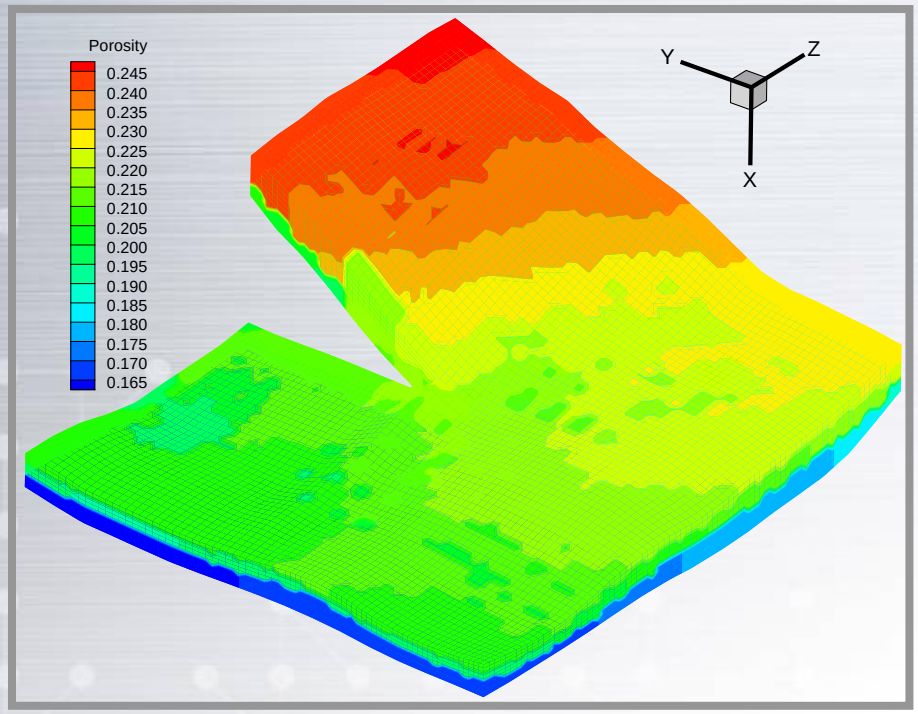
Approx. permeability field



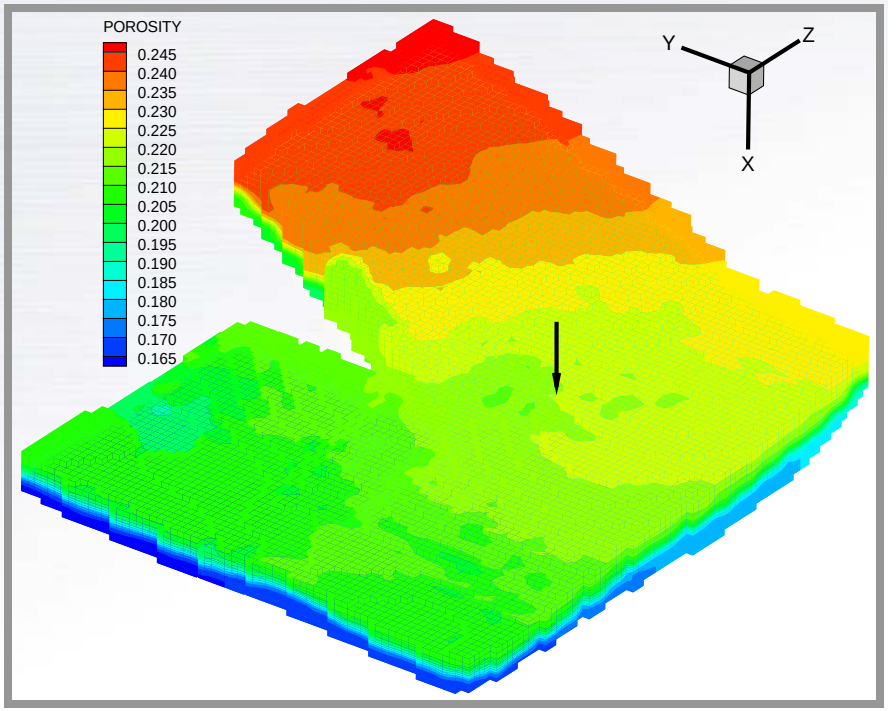
Benchmark Problem 3: Porosity

- ✓ **<u>Left</u>**: Porosity from true geometry given in a prescribed format.
- ✓ **<u>Right</u>**: Approximated porosity after interpolation onto a stair-step grid. Arrow indicated injection well location.

True porosity

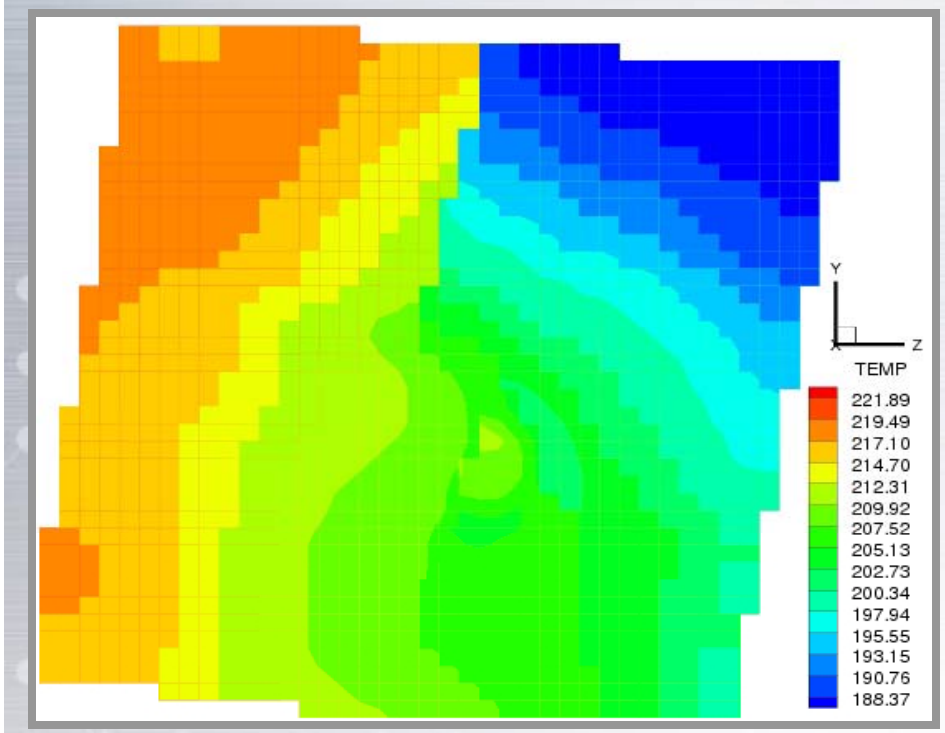


Approx. porosity

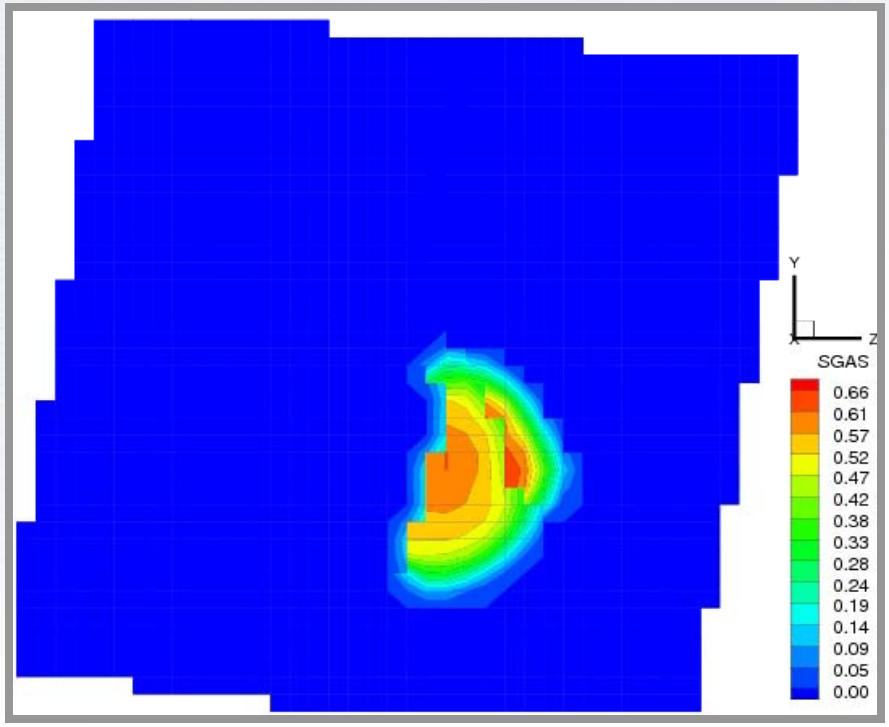


Benchmark Problem 3 Results @ 50 yrs

Temperature



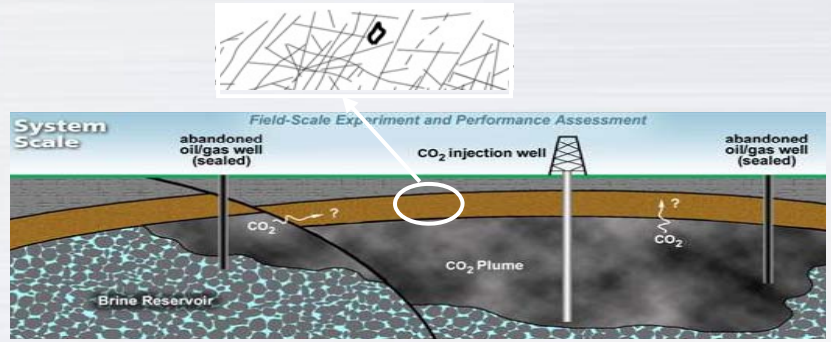
Gas Saturation



Coupled Flow and Fracture

❑**Implemented a self-adaptive quasi-static algorithm into transient dynamic pervasive fracture code**

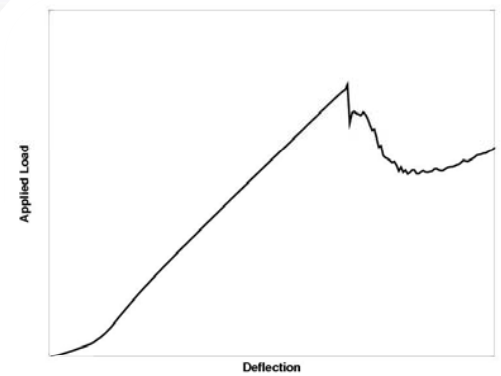
- added velocity and frequency dependent critical damping term
- adaptive Rayleigh quotient to get participating natural frequency
- mesh homogenization (uniform CFL) to transmit information uniformly throughout the mesh



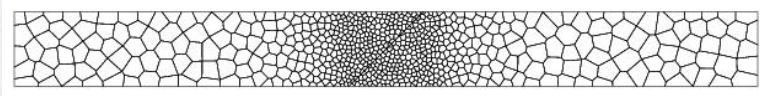
Mechanical fracturing results in CO_2 containment breach

❑**Initial assumptions made regarding fracture models**

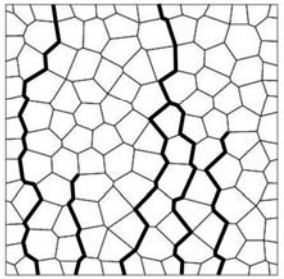
- Assume that fractures are present and initially impermeable
- Consider only fractures that run completely through the caprock
- Fractures are only allowed to reactivate along specific orientations
- Caprock material is modeled as a hyper-elastic material with a cohesive zone traction model for separation



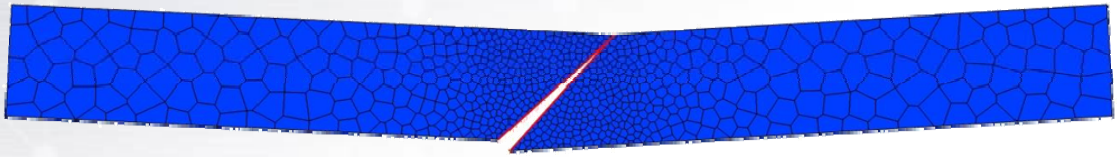
Coupled Flow and Fracture



- Analyses considered to date
  - solved single crack, variable orientation problems
  - angles 0 (vertical) to 45 degrees
  - pressure and/or displacement loading
  - elastic material response with cohesive zone model for fractures

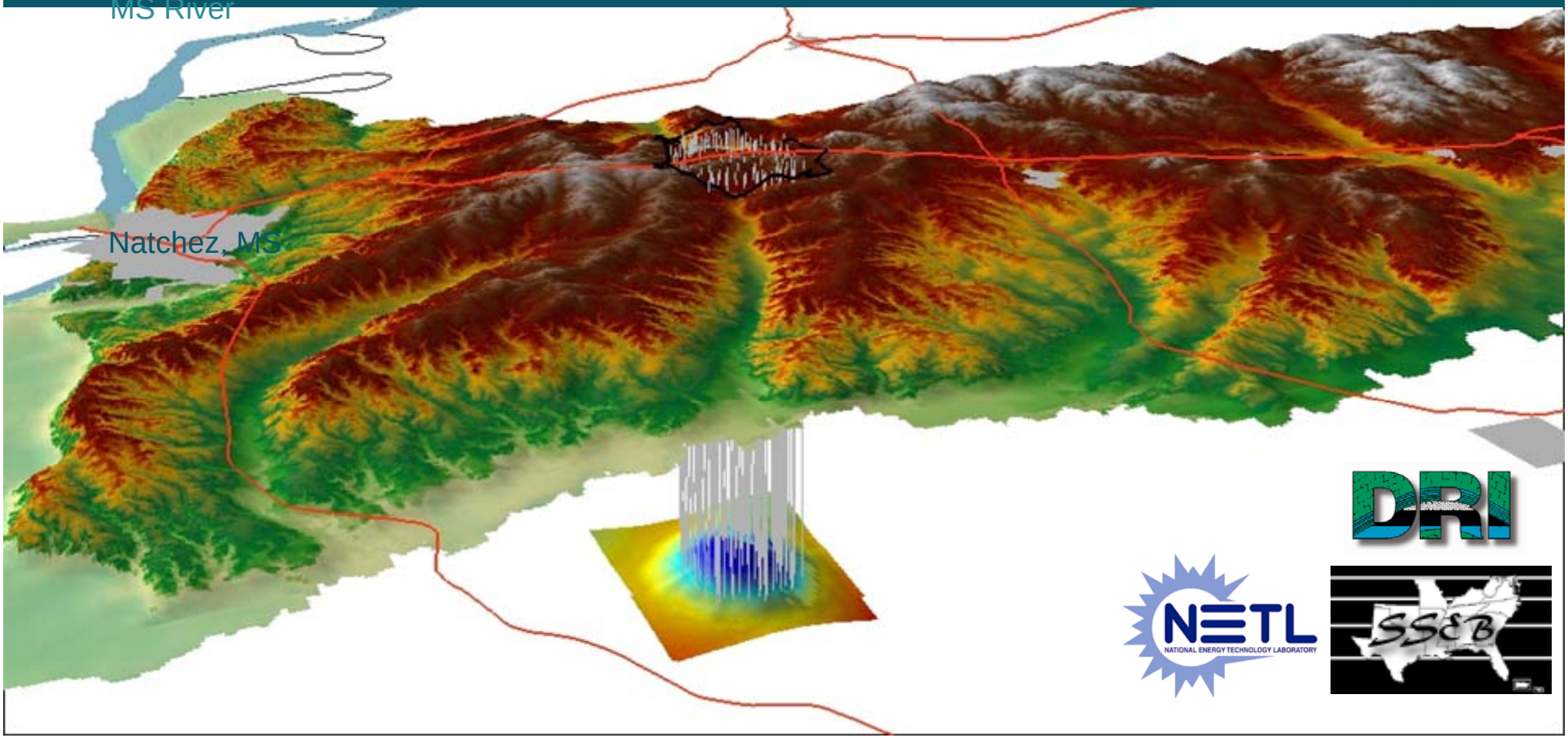


- Developed analytic porous flow solution for flow in fracture
  - quasi-steady flow initially, moving to transient (under evaluation)
  - network model based on lubrication theory
  - allows for variable aperture fractures
  - acts as pressure loading on crack faces
- Leveraged development to handle multi-sided elements into EXODUS database
- Leveraged development to get a general mesh tool for random Voronoi meshes

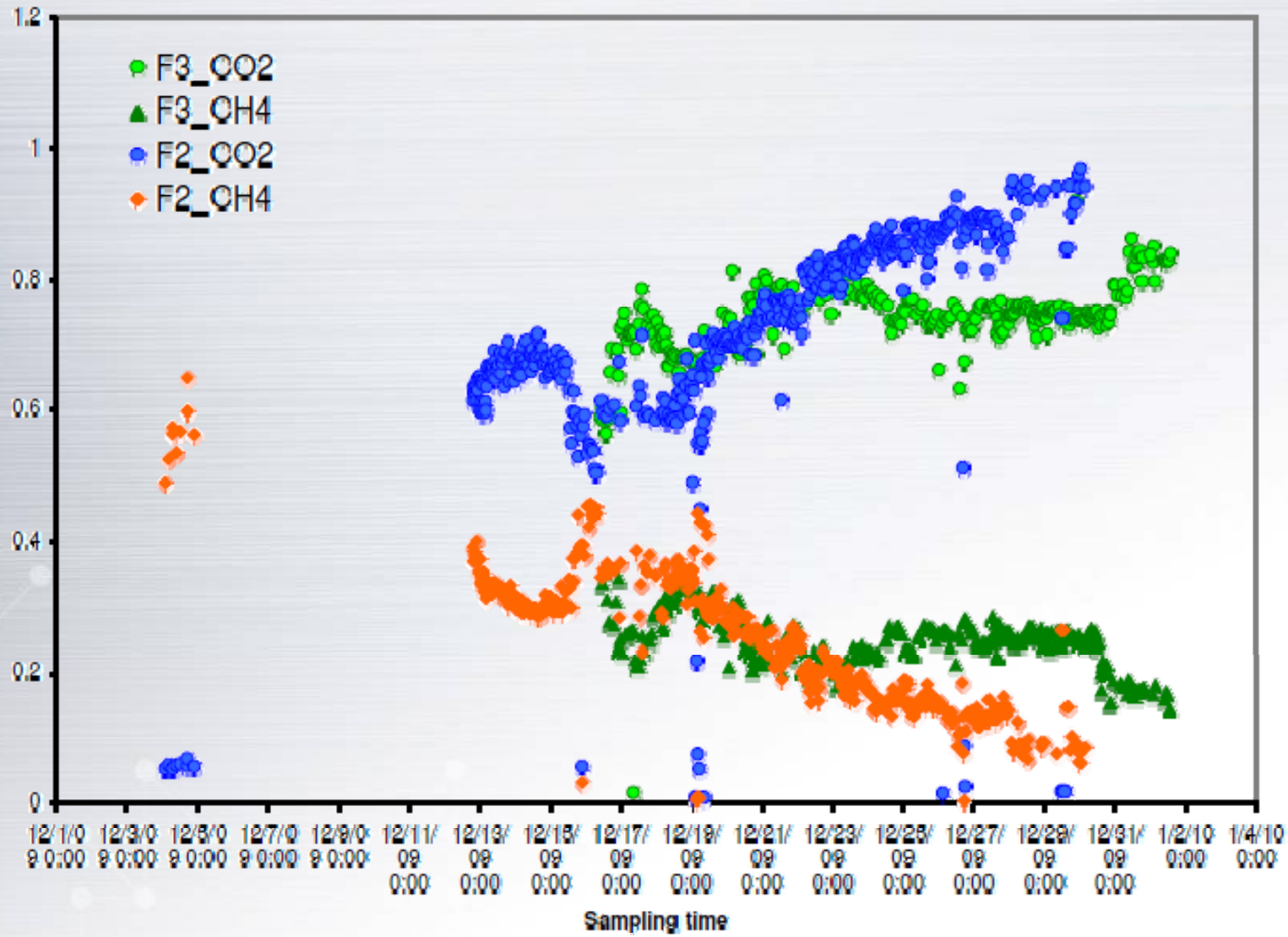


Cranfield Stacked Storage Field Test

Phase 3:
2 observation wells, multiple injectors, 1 Mt/yr
Various monitoring tools



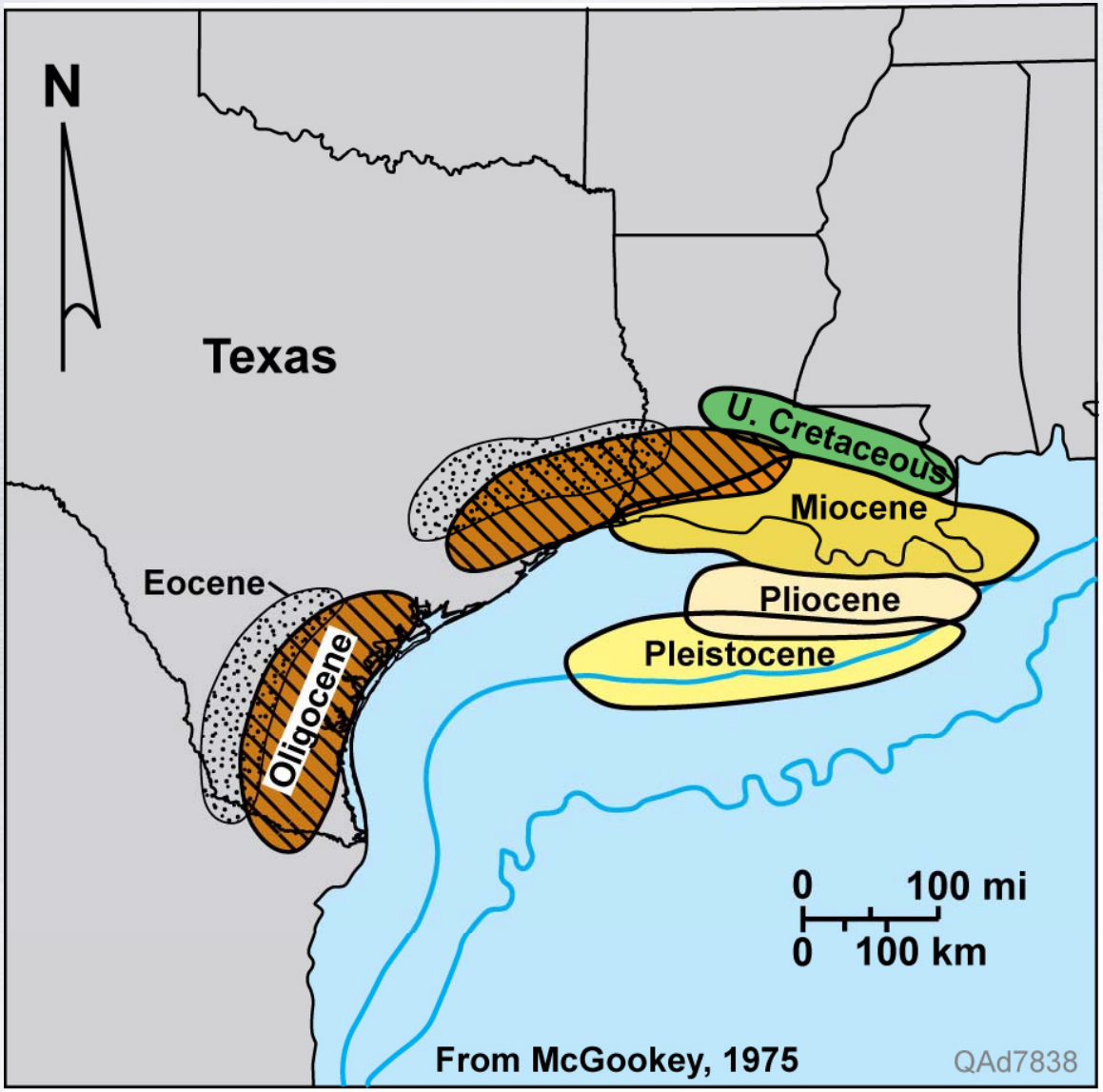
Cranfield Stacked Storage Field Test



New Approach

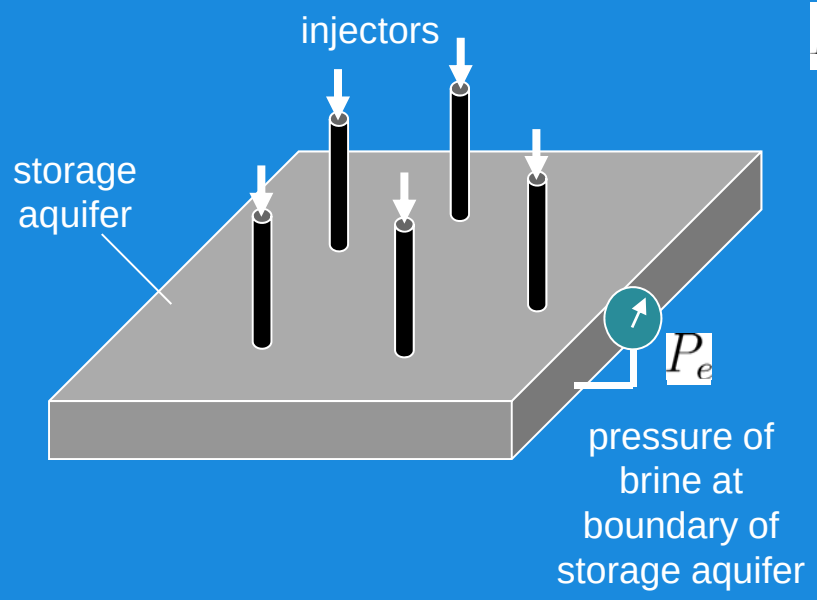
- Dissolved CH_4 is typically about 30 SCF/Bbl of brine
- Estimates of dissolved CH_4 in aquifers along the Gulf Coast range from 3000 to 46,000 TCF (Griggs, 2005) compared to 238 TCF (US proven reserves) to 1,700 TCF (US total including unconventional resources)
- In the 70s and 80s, researchers investigated geopressured aquifers saturated with methane (CH_4)
- Wells were drilled and tested
  - The Pleasant Bayou No. 2 well produced 330 MMSCF of natural gas from 1979 to 1983
  - Gladys-McCall No. 1 well produced 675 MMSCF and 27 MMbbls of water from 1983 to 1987
- When CO_2 dissolves in brine almost all of the CH_4 forms a separate gas phase

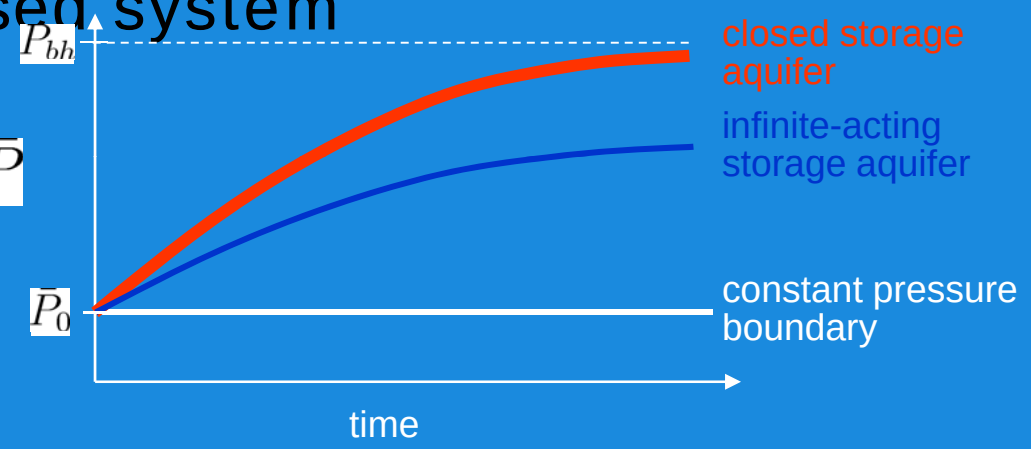
Location of Geopressured Aquifers Along the Gulf Coast

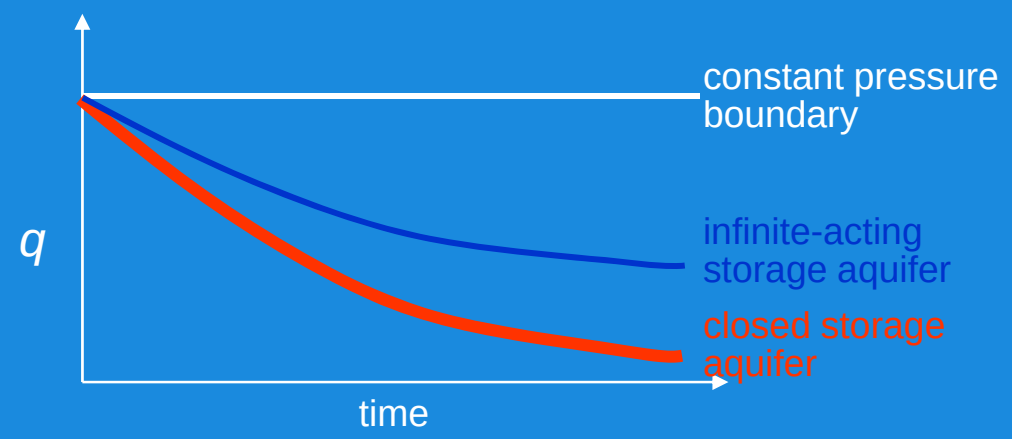


Key Limitation to Geologic CO_2 Storage: Controlling Pressure Increase During Injection

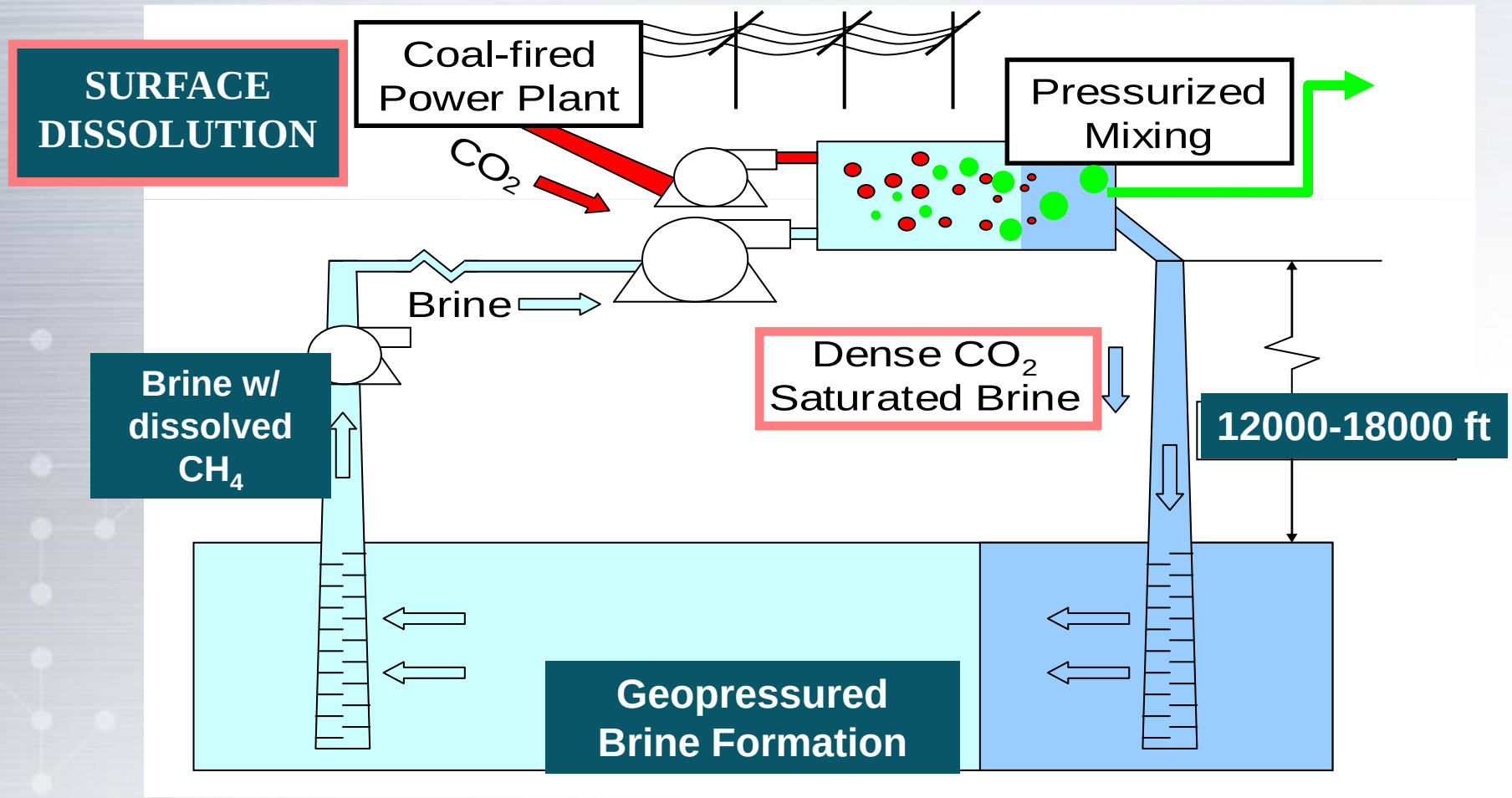
Pressure increase in aquifer is main limitation on CO_2 injection rate if there is no production and if the aquifer acts like a closed system







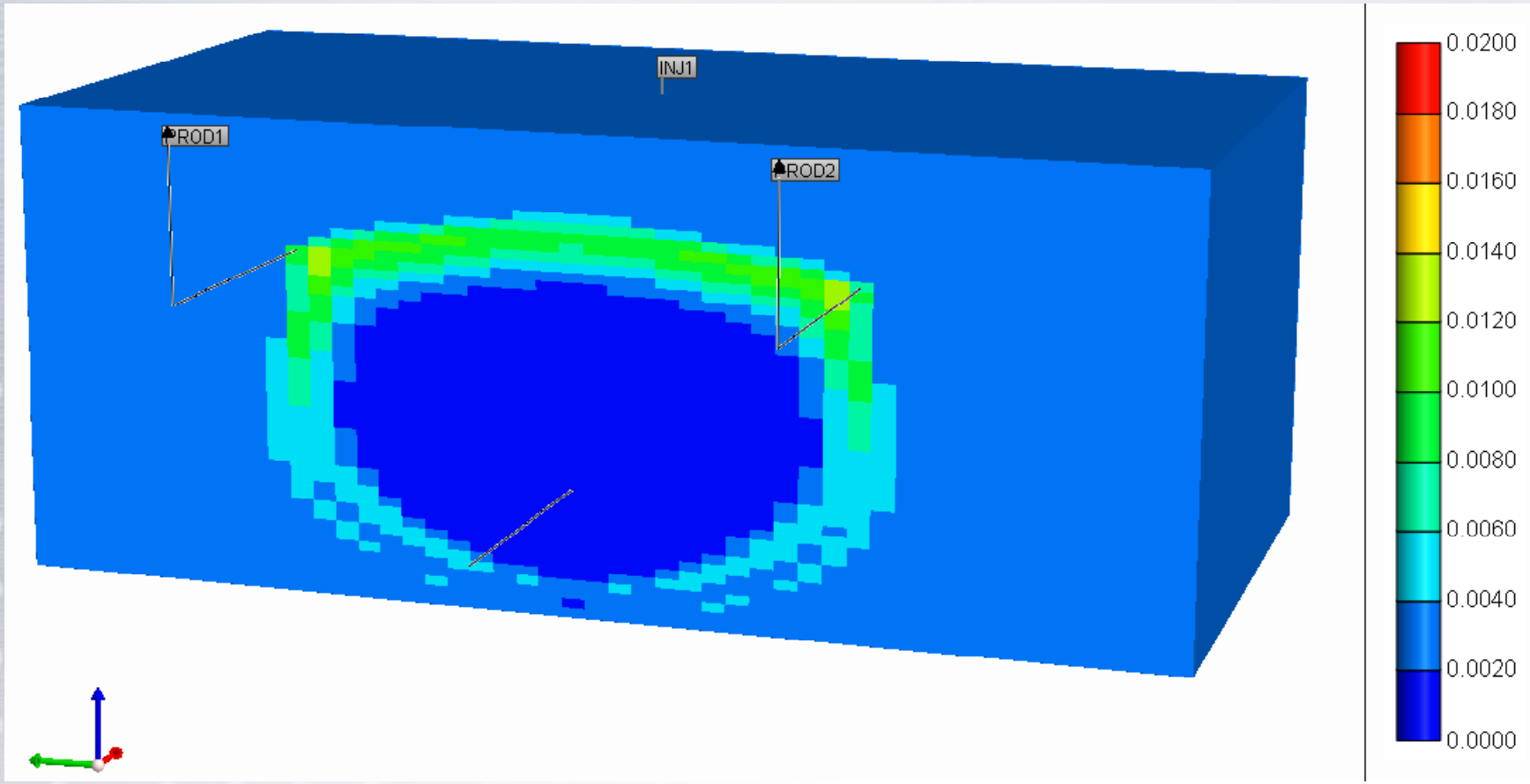
Applying the "Surface Dissolution*" Concept Provides Constant Pressure Boundary AND Reduces Injection, Compression Costs



Questions

- What fraction of the methane can be produced and at what rates
- What is the total volume of CH_4 that can be produced and the total volume CO_2 that can be stored in geopressured aquifers
- What is the best strategy for injecting CO_2 and producing CH_4
- What is the economic benefit of producing CH_4 and/or geothermal brine saturated with CH_4
- What are the most important problems

Methane bank after 730 Days



Partial List of Complications and Uncertainties

- Produced CH_4 mixed with CO_2
- Aquifer heterogeneities, faults, barriers, …
- Relative permeability hysteresis/gas trapping
- Impurities in injected CO_2
- Uncertainties in aquifer size and properties
- Pipe scaling and plugging by reservoir brine
- Uncertainties in how to operate wells
- Uncertainties in cost to operate
- Uncertainties in government regulations and incentives

CFSES External Activities

A Teacher Workshop on “The Role of Computation in Protecting the Environment: A Workshop on Carbon Sequestration Simulation for High School Mathematics and Science Teachers.”

June 15-16, 2010

hosted by

M. Wheeler, M. Delshad, T. Arbogast, and I. Duncan

Funded by NSF and DOE

Outreach Program

The Role of Computation in Protecting the Environment

Exciting and Fascinating Workshop for Science and Mathematics Educators

EDUCATORS WILL RECEIVE AN HONORARIUM FOR ATTENDING.

- Hotel accommodation will be provided for out of town participants.
- All participants will receive complimentary meals.
- Dinner on June 15th will be served on a Colorado River steam boat.

One and a half day program

Hosted by CSM and BEG at the University of Texas, and funded by the National Science Foundation's Cyber-Enabled Discovery and Innovation (CDI) program and the Department of Energy's Center for Frontiers of Subsurface Energy Security (CFSES).

TECHNOLOGY SOLUTIONS THAT PROTECT OUR INTEREST IN THE FUTURE

The workshop will inform and challenge high school educators so they can in turn impact the students under their charge. We will discuss the emerging interdisciplinary role of mathematics and computational science in the simulation and solution of the world's Grand Challenges, illustrated by the environmentally important carbon storage problem.

There will be discussions on laboratory and field experiments, mathematical modeling and large scale parallel computation. We will train attendees in the use of a sophisticated groundwater simulator as a tool to engage and pique the interest of high school students, perhaps leading some to careers in mathematics and science.

CDI & CFSES
The University of Texas at Austin

Location:
J.J. Pickle Research Campus
10100 Burnet Road, Austin, TX 78758

To ensure availability, interested people should contact the program's senior Administrator Ms. Connie Baxter connie@ices.utexas.edu
Tel 512.475.8625 Fax 512.232.2445 and
Dino Golgoon dino@mail.utexas.edu Tel 512.232.4193

Center for Subsurface Modeling (CSM), Institute for Computational Engineering & Sciences, Bureau of Economic Geology (BEG) and Institute for Geophysics
The University of Texas at Austin

TARGETING:

- High school teachers of mathematics and science
- Advanced high school students
- Undergraduate students with an interest in high school teaching

PURPOSE:

Build-up of greenhouse gases in the atmosphere, such as carbon dioxide (CO_2), is a serious environmental problem facing the global community. It is considered one of the world's Grand Challenge problems by the National Academy of Engineering, because to solve it requires both fundamental scientific progress and interdisciplinary teams of investigators working together.

A proven means of permanently preventing greenhouse gasses from entering the atmosphere is geologic sequestration. CO_2 gas is captured, perhaps from the exhaust of a fossil fuel power plant, and stored underground in large geologic saline aquifers or depleted oil fields. Predictive computational simulation may be the only means to provide an adequate assessment of the risks to public health and project failure.

The role of Computation in Protecting the Environment: A workshop on Carbon Sequestration Simulation for High School Mathematics and Science Teachers

Schedule of Events

June 15-16, 2010

Tuesday, June 15, 2010

Welcome and Opening Remarks
Greenhouse gas emissions

- World energy demand
- CO_2 buildup in the atmosphere and global warming

Geologic Sequestration

- What it is
- Where it can be done
- Where it has been done

9:45 Break
The grand challenge of carbon sequestration

- Overall challenges
  - Injectivity
  - Leakage
  - Monitoring
  - Intervention
  - Risk assessment
- Role of computational simulation

The mathematics of flow in porous media
11:45 Lunch (provided)
Numerical approximations
Reservoir simulators

2:30 Break
Tour of the laboratory facilities

- Institute of Geophysics
- Bureau of Economic Geology
- Texas Advanced Computing Center

Dinner will be provided on the Colorado River

Wednesday, June 16, 2010

Field experiments
Mathematical modeling of CO_2 processes
9:45 Break
Field –scale CO_2 simulation
Parallel processing
11:45 Lunch (provided)
UT-Chem, a groundwater simulator
Concluding remarks

UT Faculty and Staff

- Mary Wheeler
- Todd Arbogast
- Mojdeh Delshad
- Ian Duncan
- Tim Wildey

CDI & CFSES
The University of Texas at Austin

SciDAC-e Projects

Patrick Knupp : “Mesh generation for modeling and simulations of carbon sequestration processes”

Michael Heroux: “Algebraic multi-grid methods for modeling, simulation and uncertainty quantification of carbon sequestration processes on multi-core architectures”