



Validation of Models Simulating Capillary and Dissolution Trapping During Injection and Post- Injection of CO₂ in Heterogeneous Geological Formations Using Data from Intermediate Scale Test Systems (FE0004630)

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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



Presentation Outline



- Benefit to the Program**
- Project Overview**
- Technical Status**
 - **Task 2 – Intermediate-scale laboratory testing of capillary and solubility trapping in homogeneous and heterogeneous systems**
 - **Task 3 – Evaluation of whether existing modeling codes can capture the processes observed in the laboratory, and developments of the constitutive models based on the findings**
- Accomplishments to Date**
- Project Summary - Findings and Future Plans**
- Appendix**

Benefit to the Program



❑ Overall Project Goals

- ❑ **Improve/develop and validate models** by using the data generated in intermediate-scale laboratory test systems simulating capillary and dissolution trapping under various heterogeneous conditions.
- ❑ Design **injection strategies, predict storage capacities and efficiency** for **field-scale** geological systems by using the improved numerical tools

- ❑ The findings will meet objectives of Program research to develop technologies to cost-effectively and safely store and monitor CO₂ in geologic formations and to ensure storage permanence. Developed approach and technologies in this project specifically contribute to the Carbon Storage Program's effort of supporting industries' **ability to predict geologic storage capacity to within +/- 30 percent.**

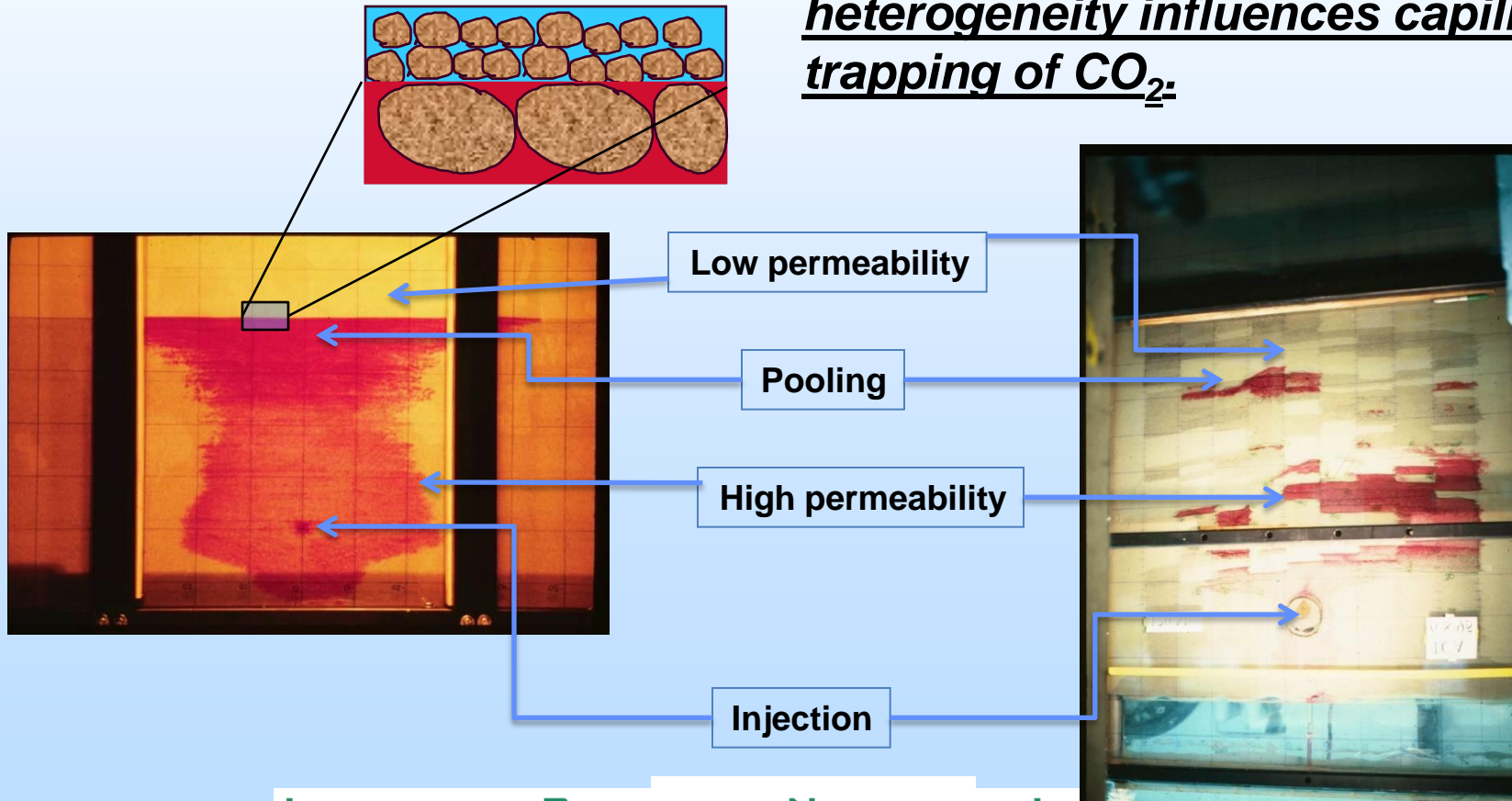
Knowledge gaps and research questions

Heterogeneity and Capillary Trapping



In naturally **heterogeneous** formations, injected scCO₂ will **preferentially migrate** into higher permeability zones and **pool under the interface** of the confining low permeability layers due **to capillary barrier effects** (very high entry pressure).

Knowledge gaps exist on how the heterogeneity influences capillary trapping of CO₂:



Heterogeneity and Dissolution Trapping



Dissolution of CO_2 in **heterogeneous** systems can be enhanced due to **increases in interfacial areas** between water and supercritical CO_2 .

*Knowledge gaps exist on how the **heterogeneity** influences dissolution trapping of CO_2 .*



Capillary Trapping

- ❑ How do **heterogeneities and connectivity (spatial continuity of different permeability zones)** affect entrapment efficiency of scCO_2 in deep geological formations?
- ❑ How well the **existing continuum-based models and the constitutive models** capture multiphase flow behavior of scCO_2 /brine in deep formations?

Dissolution Trapping

- ❑ What are the **effects of heterogeneity** on dissolution and **density-driven fingers**?
- ❑ Can dissolution of CO_2 in **heterogeneous systems** be enhanced due to increases in **interfacial areas** between water and supercritical CO_2 ?

Project Objectives and Tasks



- Task 1 – Project Management and Planning
- **Task 2 – Generate data** in intermediate scale test tanks simulating **capillary trapping and dissolution** affected by **heterogeneity**
 - Task 2.1 – Small tank experiments
 - Task 2.2 – Large tank experiments
- **Task 3 – Evaluate** whether the **existing modeling codes** can capture processes observed in the test tanks, and **improve** existing models based on findings

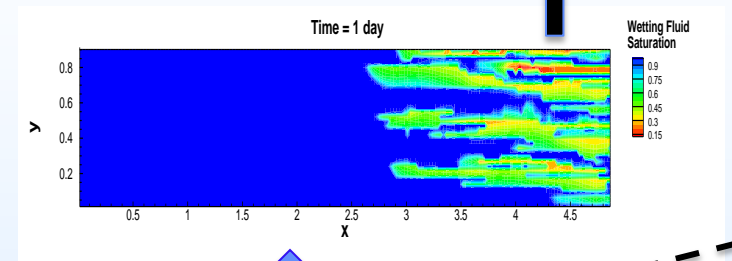
Approach



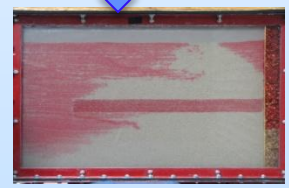
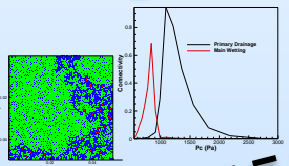
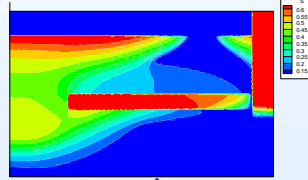
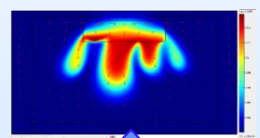
A multi-scale experimental testing and modeling

Upscaling → Field Scale

LBNL



Upscaling →



Intermediate-Scale

← 1 to ~ 10 m →

CESEP
Center for Experimental Study of Subsurface
Environmental Processes

Size (cm to basin scale)

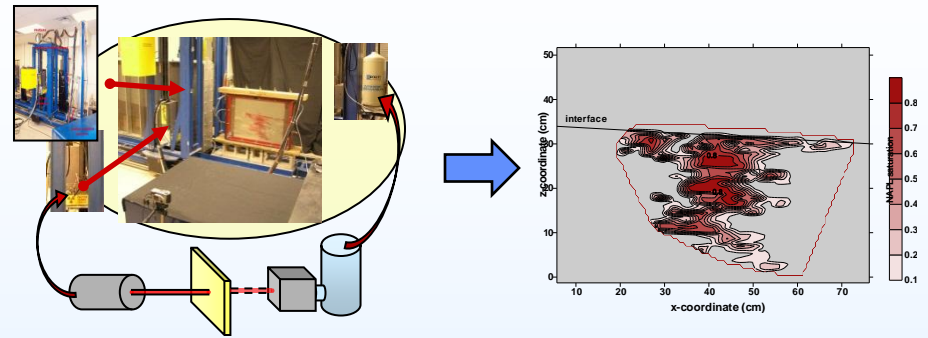
LAWRENCE BERKELEY NATIONAL LABORATORY

Model Dimension ↑

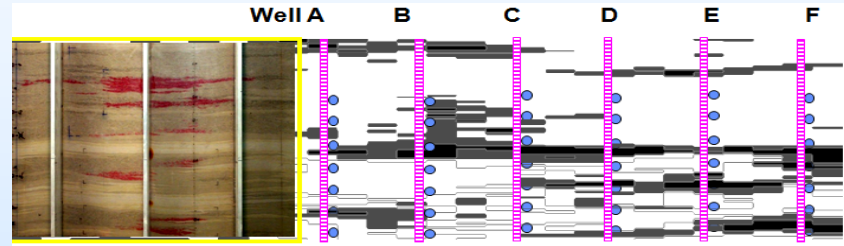
Experiment Dimension ↑

Experimental Methods

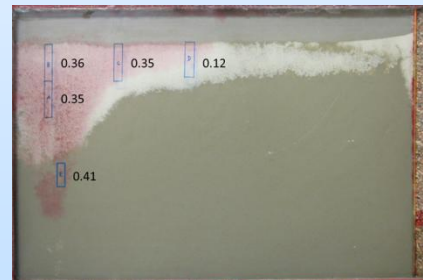
❑ Automated transient and spatially distributed saturations using x-ray attenuation



❑ Aqueous sampling to determine dissolved plume concentrations, and core destructive sampling from low permeability zones



❑ Core destructive sampling to determine final entrapment saturations.



❑ Measurement of multiphase model parameters (capillary pressure-saturation-relative permeability relationships)



Task 2 – Experimental Studies



❑ Selection of materials and fluids

- ✓ Dimensional analysis (Bo , Ca , density and viscosity ratio, Ra number)
- ✓ Small test systems in fluid/fluid media and small sand tanks (28cmx15cm)

❑ Small tank experiments (28cmx15cm and 92cmx1.2m)

- ✓ Capillary trapping in homogeneous and simple heterogeneous packing (8 experiments completed)
- ✓ Analyses of density-driven finger developments in homogeneous and heterogeneous packing (4 experiments completed)
- Capillary trapping in highly heterogeneous systems (in progress)
- Capillary and dissolution trapping (homogeneous and heterogeneous packing)

❑ Large tank experiments (4.9mx1.2m)

- Capillary trapping (in progress)
- Capillary and dissolution trapping

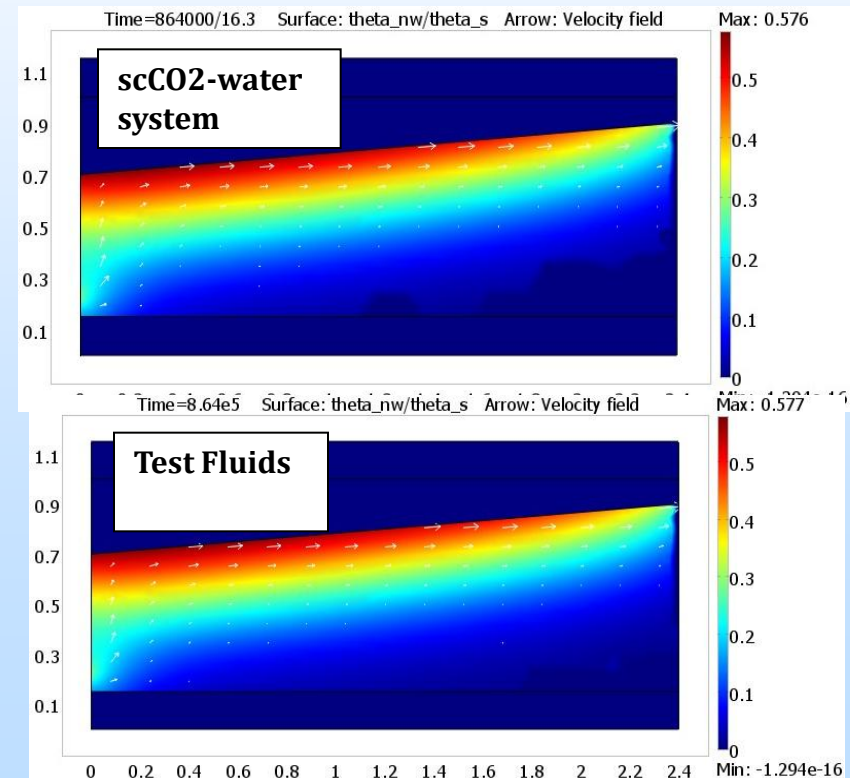
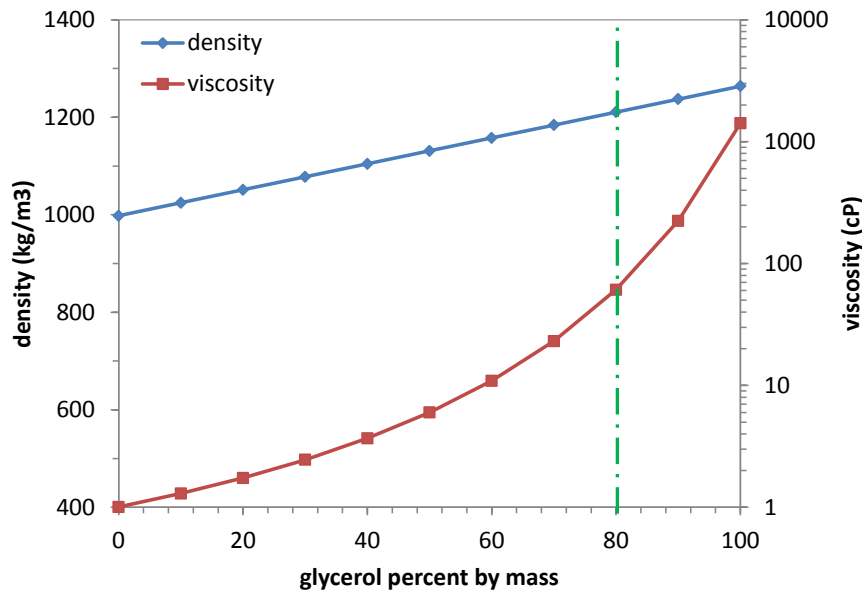
- Laboratory investigation of scCO₂ migration without high pressure can be conducted using **analogous fluids having similar density and viscosity contrasts as scCO₂ – brine phases** under sequestration conditions

Dimensionless Numbers	scCO ₂ -brine @ Typical Reservoir Conditions	Soltrol220-glycerol/water @ 20C, 1 atm	Water in Propylene Glycol @ 20C, 1 atm	Methanol in glycerol/water @ 20C, 1 atm
Bond # $B_o = \frac{\Delta\rho g k}{\sigma}$	~ 10 ⁻⁷ - 10 ⁻⁸	~10 ⁻⁶ - 10 ⁻⁷	~10 ⁻⁶ - 10 ⁻⁷	~10 ⁻⁶ - 10 ⁻⁷
Capillary # $Ca = \frac{\mu_{nw} u_T}{\sigma}$	~ 10 ⁻⁵ - 10 ⁻⁸	~10 ⁻⁶ - 10 ⁻⁷	~10 ⁻⁷ - 10 ⁻⁸	~10 ⁻⁷ - 10 ⁻⁸
Viscosity Ratio $\frac{\mu_{nw}}{\mu_w}$	~ 0.05 - 0.2	~0.074	~0.017	~0.07
Density Ratio $\frac{\rho_{nw}}{\rho_w}$	~ 0.2 – 0.8	~0.66	~0.9	~0.6

Testing of the Scaling Approach

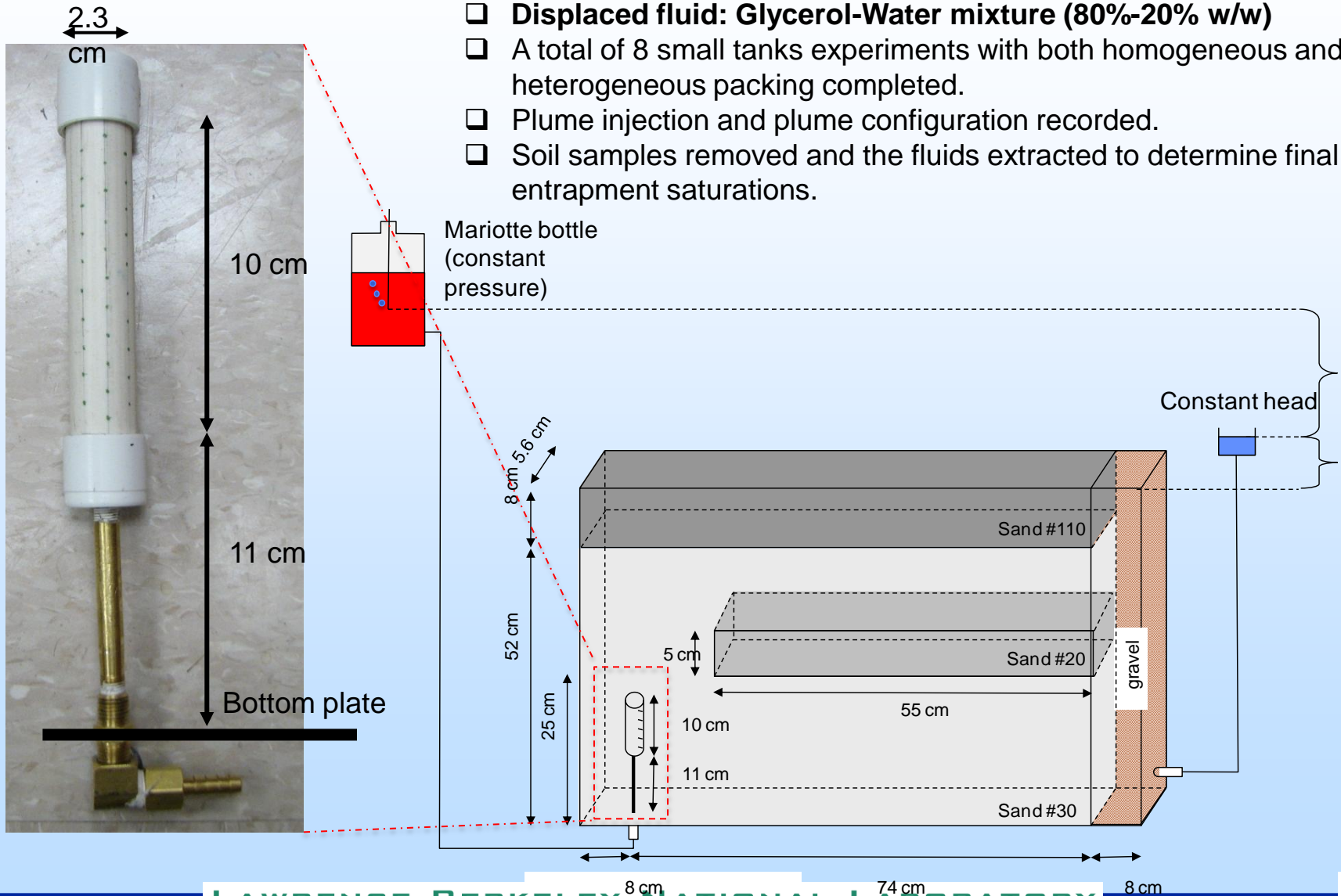
- Identical results can be obtained if the same dimensionless numbers are chosen for the geometrically similar two systems (Shook et al., 1992; Gharbi et al., 1998).

Glycerol/water mixture at ambient conditions



Small Tank Experiments For Capillary Trapping in Homogeneous and Heterogeneous Systems

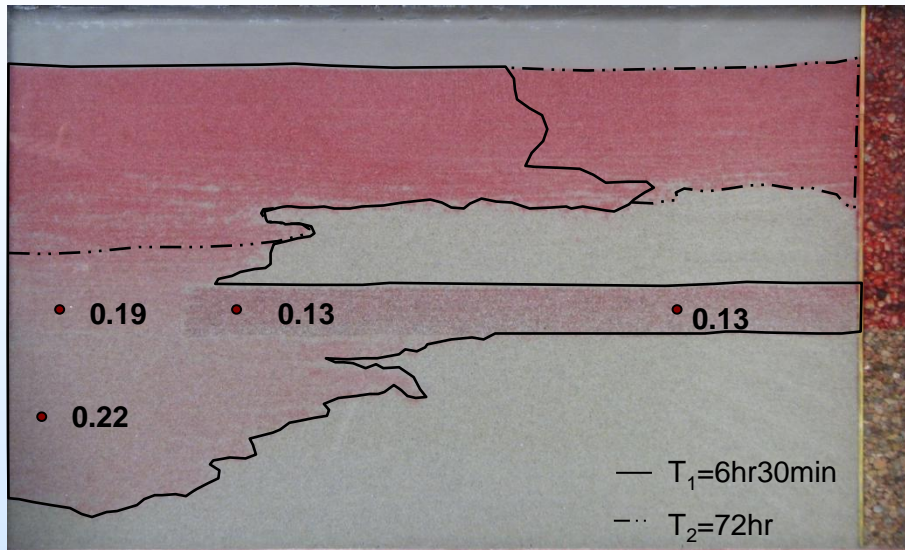
- ❑ Injected fluid: **Soltrol 220**
- ❑ Displaced fluid: **Glycerol-Water mixture (80%-20% w/w)**
- ❑ A total of 8 small tanks experiments with both homogeneous and heterogeneous packing completed.
- ❑ Plume injection and plume configuration recorded.
- ❑ Soil samples removed and the fluids extracted to determine final entrapment saturations.



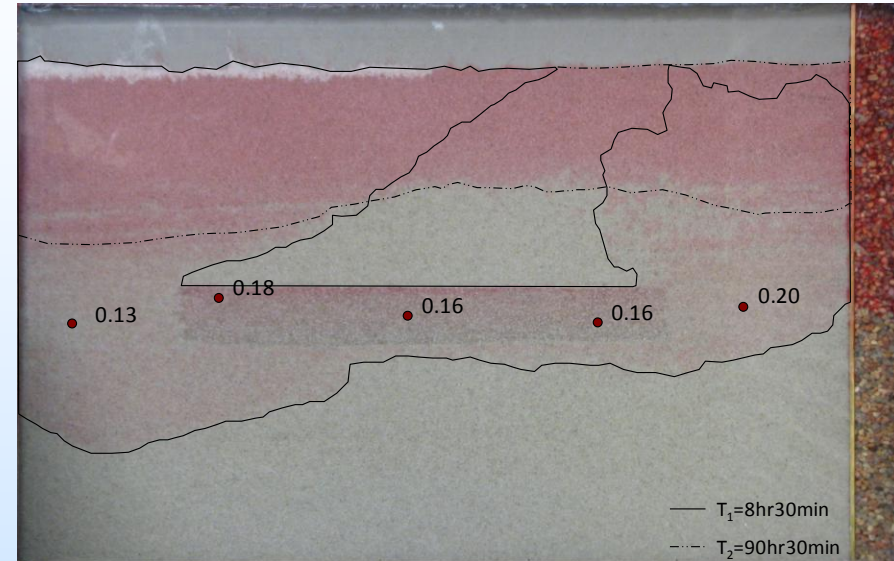
Small Tank Experiments for Capillary Trapping in Mildly Heterogeneous Systems



Heterogeneous with a continuous high-permeability layer



Heterogeneous with a discontinuous high-permeability layer

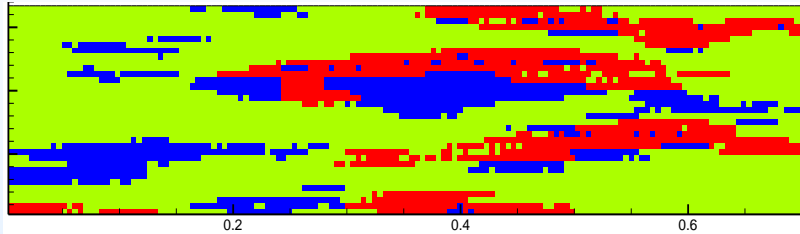


- ❑ Can models that use macroscopic multiphase parameters capture the flow and entrapment behavior ?
- ❑ Are the relative permeability models generated from retention functions adequate?
- ❑ What are the effects of injection rates (entrapment zone development and final entrapment saturations) ?
- ❑ Does the final entrapment depend on rate of injection?



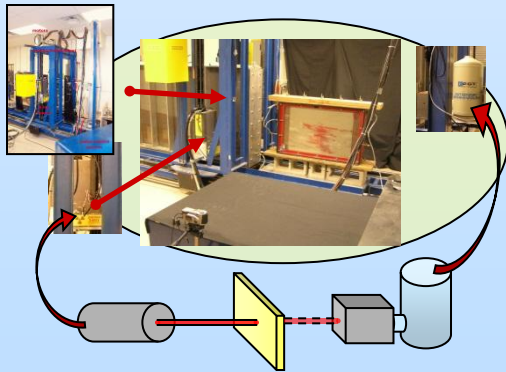
Small Tank Experiments in Highly Heterogeneous Systems (in progress)

A computer-generated realistic heterogeneous aquifer



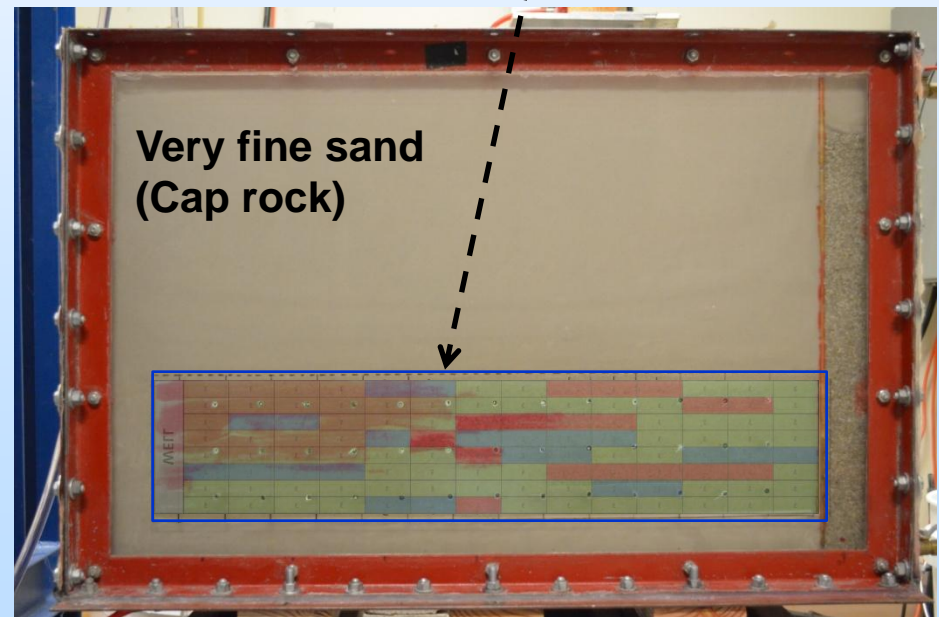
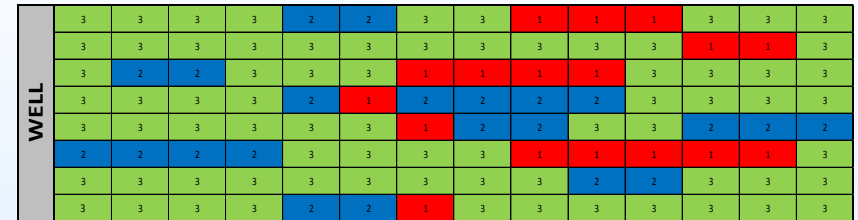
red (#30) green (#50) blue (#70)
Coarse Medium Fine

Repair of X-ray systems will be completed at the end of August



For phase saturation measurement

Simplified for packing



Small-Tank Experiments: Heterogeneity effect on density-driven fingering (water/propylene glycol)

04/13/2012 12:30pm (28 days later)



- ✓ Fingering is dampened out by heterogeneity
- ✓ From high permeability medium to low permeability medium, finger flow is replaced by bulk flow

Large Tank Experiments (in progress)

- ✓ Problems encountered in early design of the 16ft large tank experiment were mostly resolved

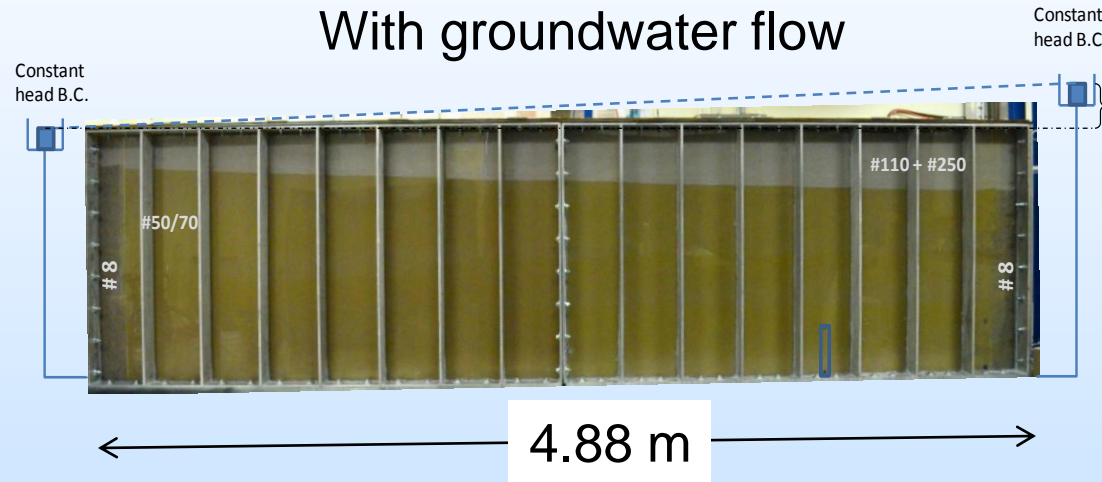
Previous



- Well configuration => non-wetting phase moves upward inside the well; only top portion of the screen injects Soltrol into the aquifer (reduced vertical sweep)
- Difficulties to avoid preferential pathway between confining layer and gasket

Current Setup for the Large Tank Experiments

With groundwater flow



❑ Guiding the laboratory experiments

- ✓ Injection rate and period, sampling frequency, different packing configurations, and effect of different boundary conditions; *i.e.*, constant head versus no flow.

❑ Testing continuum models and upscaling methodologies

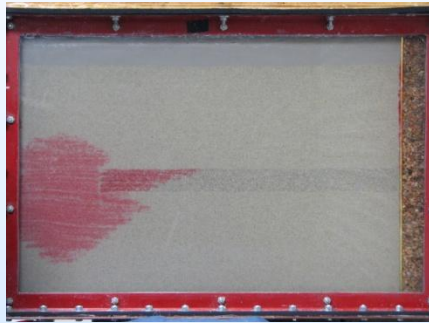
- ✓ Verify models (numerical codes solving classical two-phase flow equations) based on experimental measurements in homogeneous and heterogeneous experiments
- Test/develop constitutive models for accurate prediction of the CO₂ entrapment
- Utilize improved modeling and up-scaling tools to predict the effective capillary and dissolution trapping at actual reservoir conditions and large scale CO₂ storage scenarios
- Design injection strategies to optimize CO₂ trapping.

Model Testing

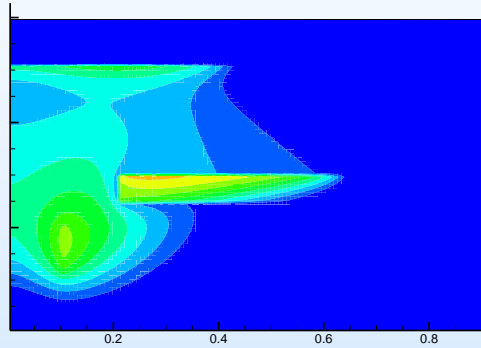
- Small tank experiment in a mildly heterogeneous domain with a continuous high-permeability zone – During Injection

Time

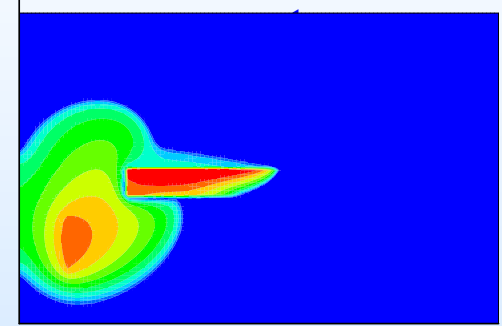
2 hr



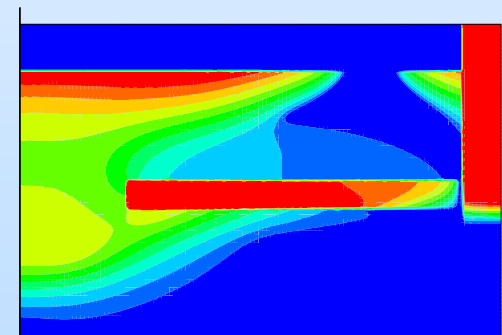
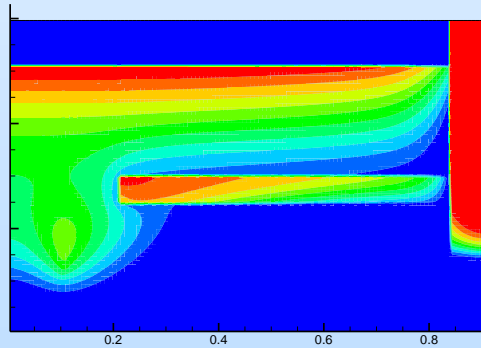
VG-Mualem & Corey



Relative perm. from Previous Results in Air-water Exp.

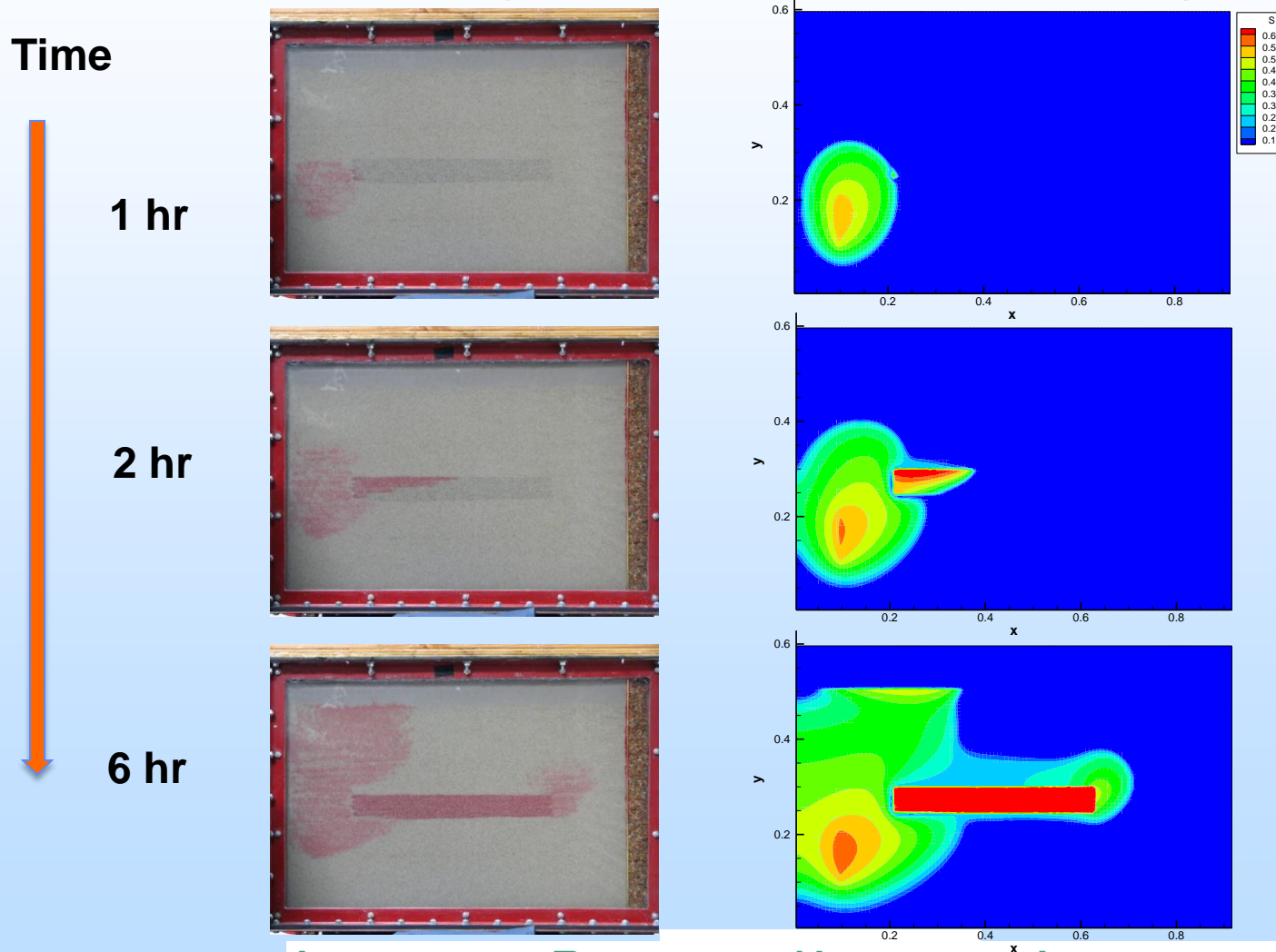


7.5 hr



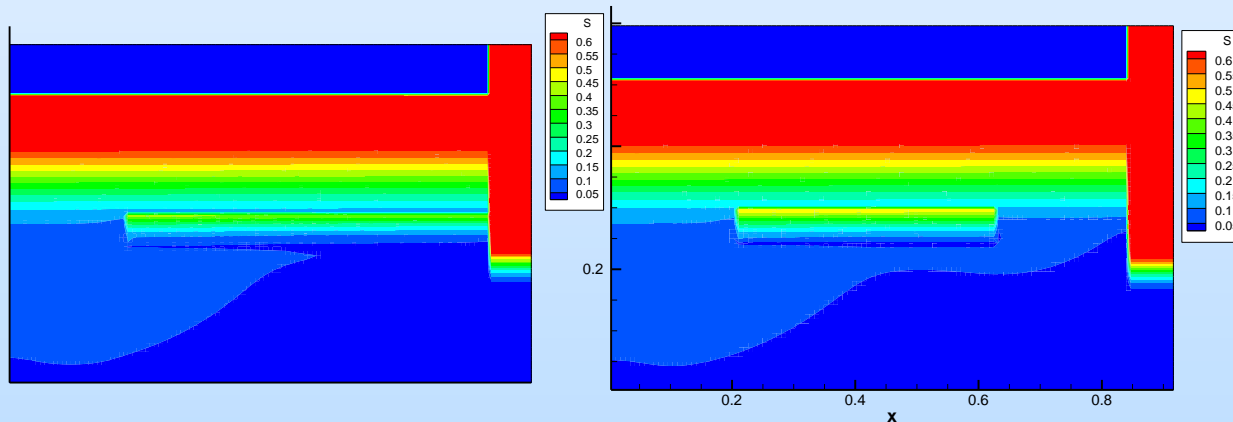
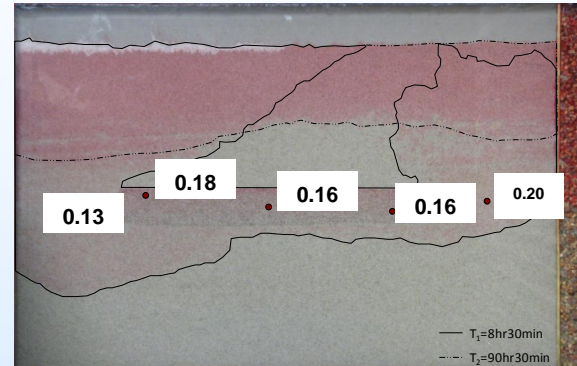
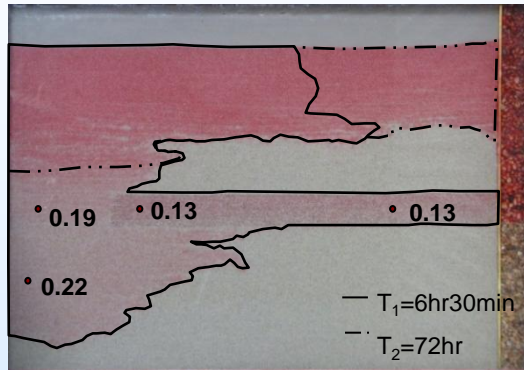
Model Testing

- Small tank experiment in a mildly heterogeneous domain with a discontinuous high-permeability zone – During Injection



Saturation distributions at the end of the experiments

Simple Heterogeneous Packing



Two-phase model results with hysteresis effects

Development of a Theoretical Hysteresis Model



Void Sizes $r_1 > r_2 > \dots > r_n$

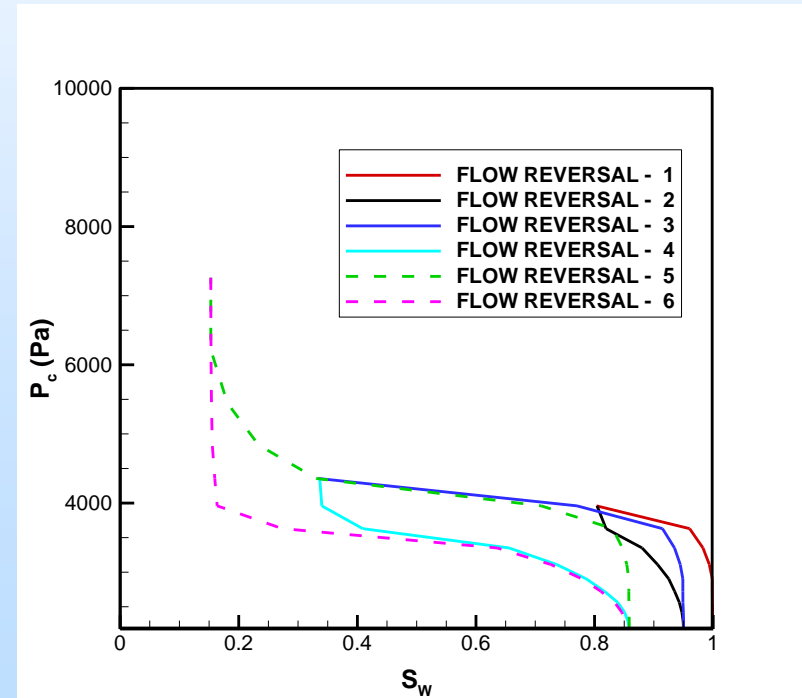
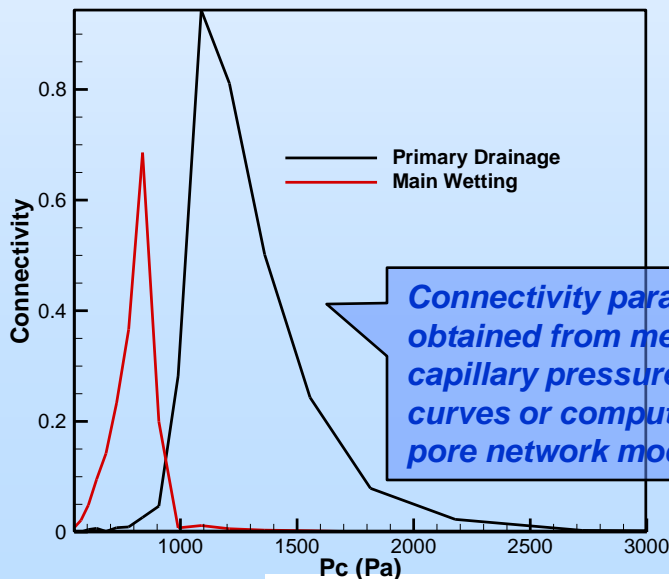
Volume Fractions f_1, f_2, \dots, f_n

Drainage
$$S_{nw}(P_{c,m}) = \sum_{i=1}^m \sum_{j=i}^m f_j p_{ij}^d \prod_{k=i}^{j-1} (1 - p_{ik}^d); \quad P_{d,m} \leq P_c, m=1,2,\dots,n$$

Imbibitions
$$S_{nw}(P_{c,m}) = S_{nw}(P_{c,n}) - \sum_{i=m}^n f_i' \left[\sum_{j=m}^i p_{ij}^w \prod_{k=j+1}^i (1 - p_{ik}^w) \right]; \quad P_{d,m} > P_{c,m}, m=n, n-1, \dots, 1$$

$$f_i' = f_i \left[\sum_{l=i}^n p_{il}^d \prod_{k=i}^{l-1} (1 - p_{ik}^d) \right]$$

Represents the fraction of pores filled with non-wetting phase at the end of drainage



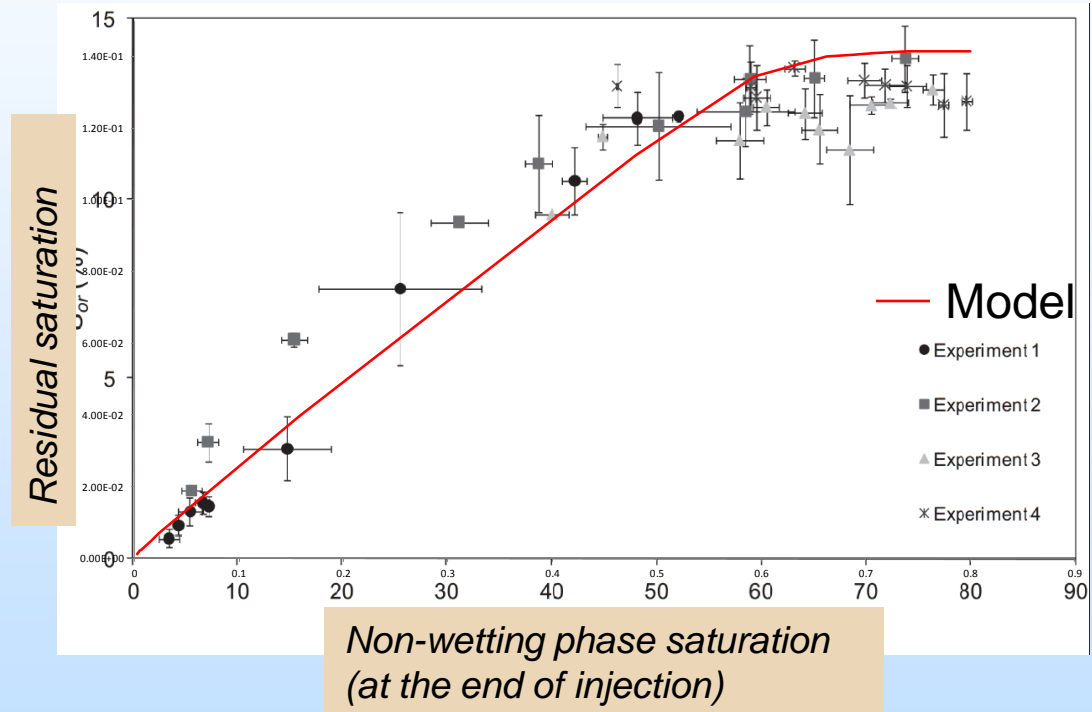
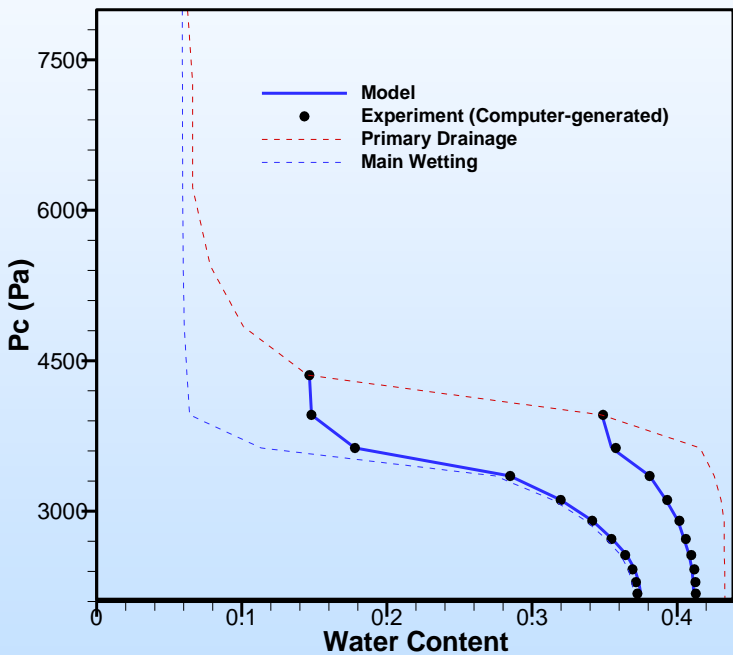
Preliminary Results

Verification of the Hysteresis Model



With computer-generated data

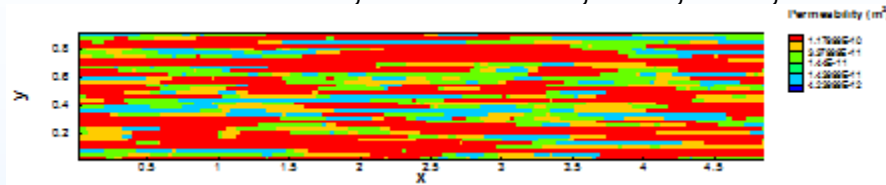
With laboratory experiments in LV60 sand with Octane/brine
(*Pentland et al. 2010*)



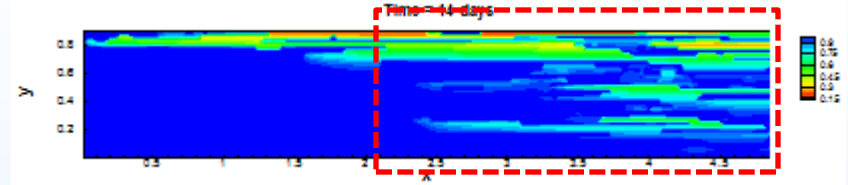
Modeling in the Large Tank and Effect of Heterogeneity



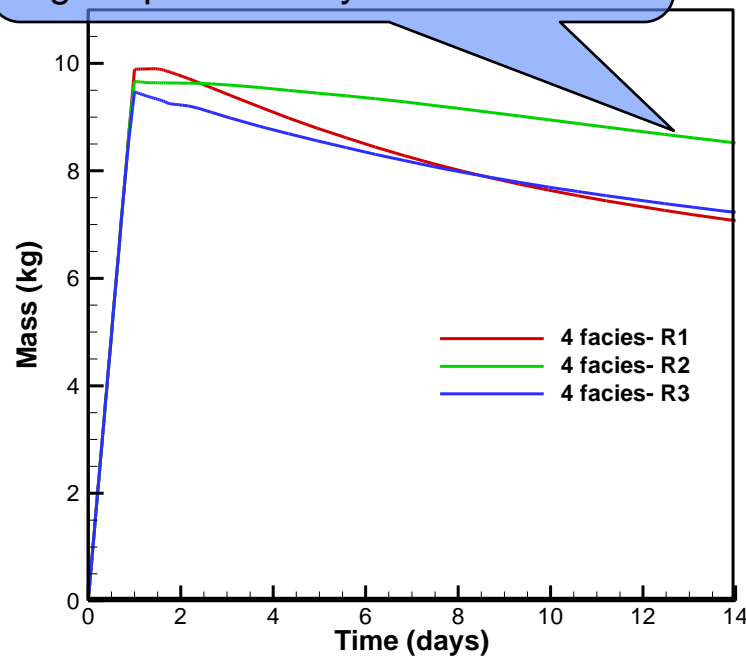
Four-Facies Case, Sands #30, #50, #70, #110



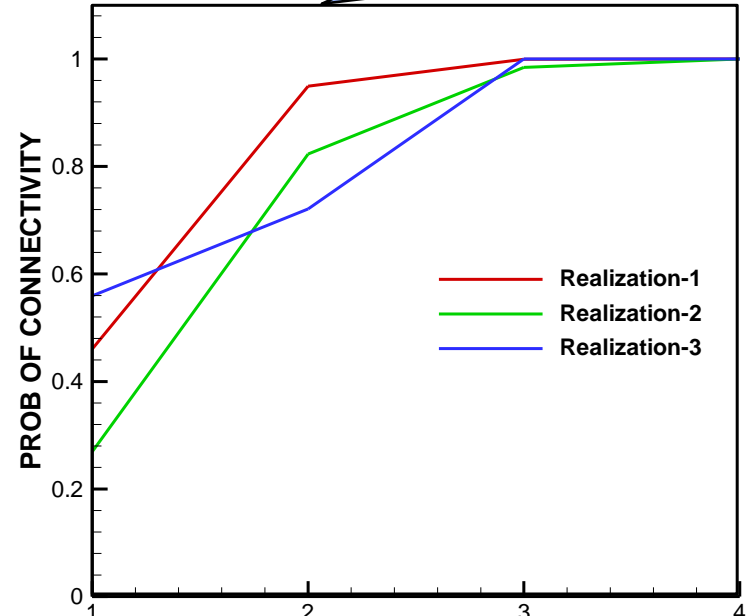
Control Volume



More mass retained in Realization-2 as a result of less connectivity of higher-permeability zones

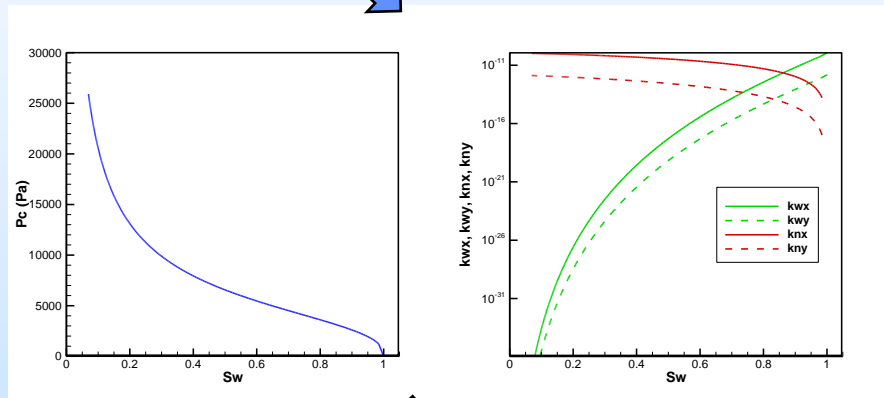
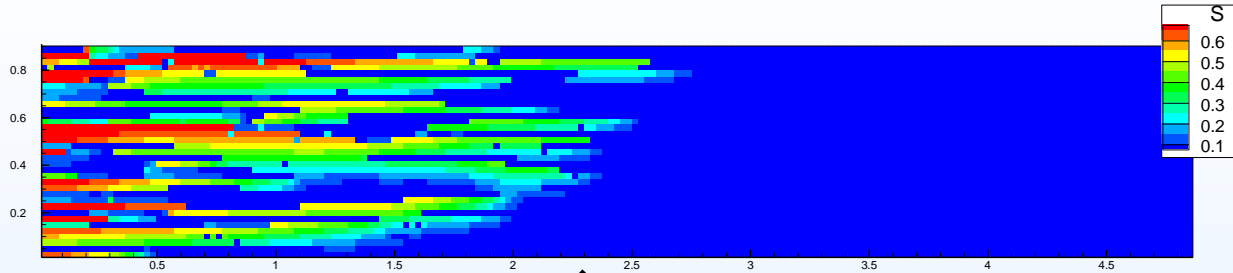


Large-scale capillary entrapment affected by connectivity!

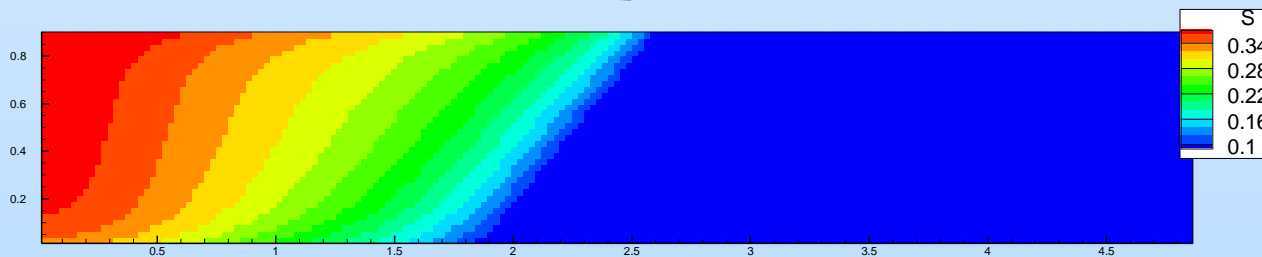


Higher k → Lower k

Model Simplification Through Upscaling



**Effective
Constitutive
Relationships**



❑ Task 2 – Experiments in intermediate-scale

- ✓ Selected and tested surrogate fluids
- ✓ Small tank experiments completed for testing capillary trapping and density-dependent fingers in homogeneous and simple heterogeneous systems
- ✓ Initiated large tank experiments for capillary trapping

❑ Task 3 – Modeling

- ✓ Developed a multiphase flow solver (based on the Finite Volume method) for analysis of the experimental data and new constitutive models and non-equilibrium mass transfer
- ✓ Simulated the two-phase flow in small tank experiments and compared the model results with experimental data
- ✓ Developed a new code for analyzing heterogeneity: Computes connectivity based on invasion percolation algorithm. This code also involves algorithms to upscale two-phase flow parameters.
- ✓ Developed a new hysteresis model and tested against few data sets

Findings

- ❑ The numerical model based on the classical two-phase flow theory was able to capture the main features observed during the migration of the CO₂ surrogate fluid in the small tanks
- ❑ Incorporating hysteresis effects into the numerical models required for accurate prediction of post-injection capillary entrapment.
- ❑ Intermediate-scale heterogeneity (existence of lower and higher permeability zones) enhances the capillary entrapment.
- ❑ Density-driven convective mixing in highly heterogeneous formations may not be important.

Future Efforts

- ❑ Obtain quantitative data on temporal and spatial saturation changes using the X-ray system
- ❑ Complete measurements of relative permeability of the sands in separate homogeneous column tests
- ❑ Update the model results in the small tank with measured relative permeability curves in separate homogeneous column tests
- ❑ Intermediate-scale heterogeneous experiments and models involving both capillary and dissolution trapping.
- ❑ Improve the numerical models by incorporating the validated constitutive models

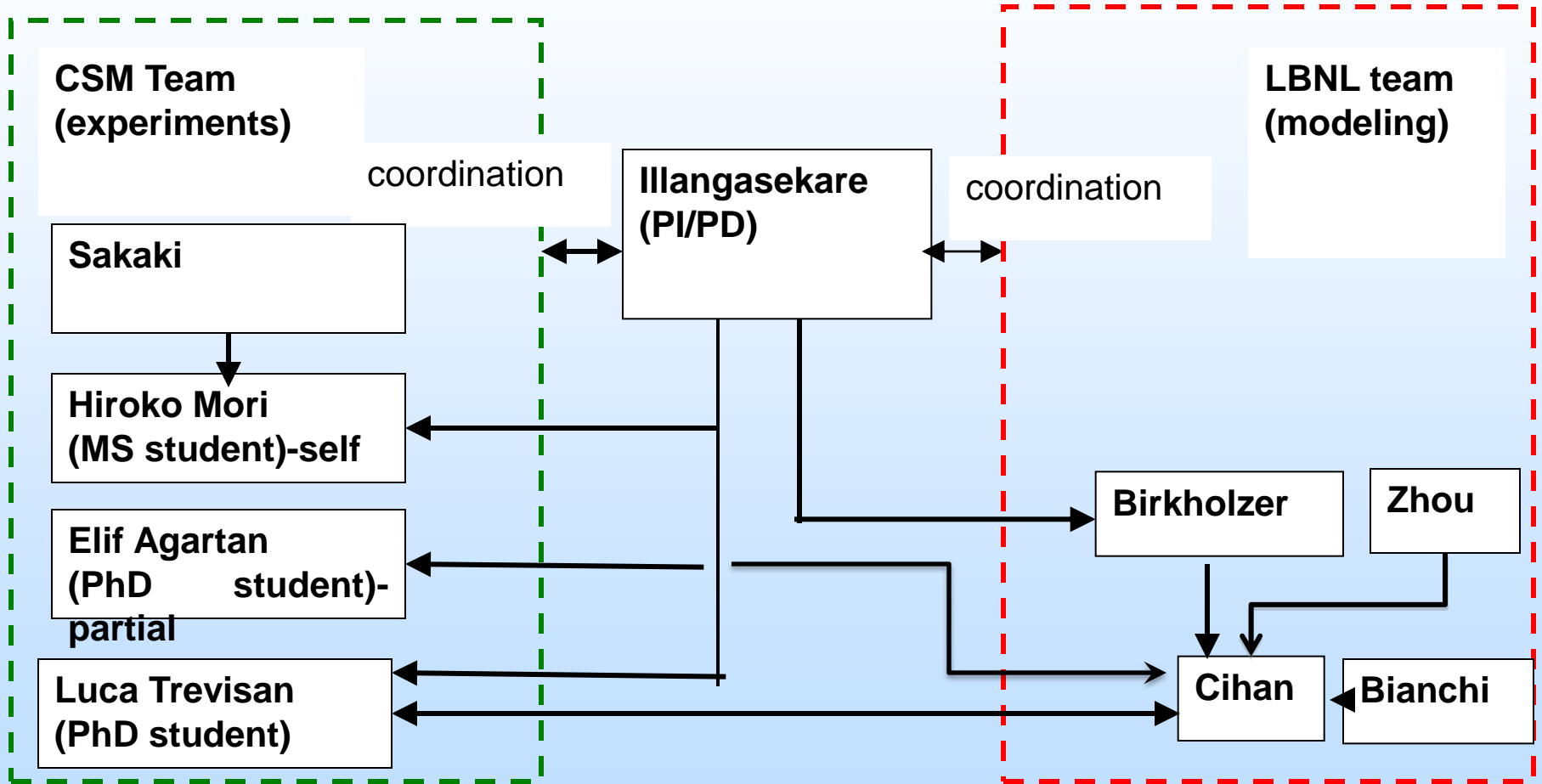
Questions?



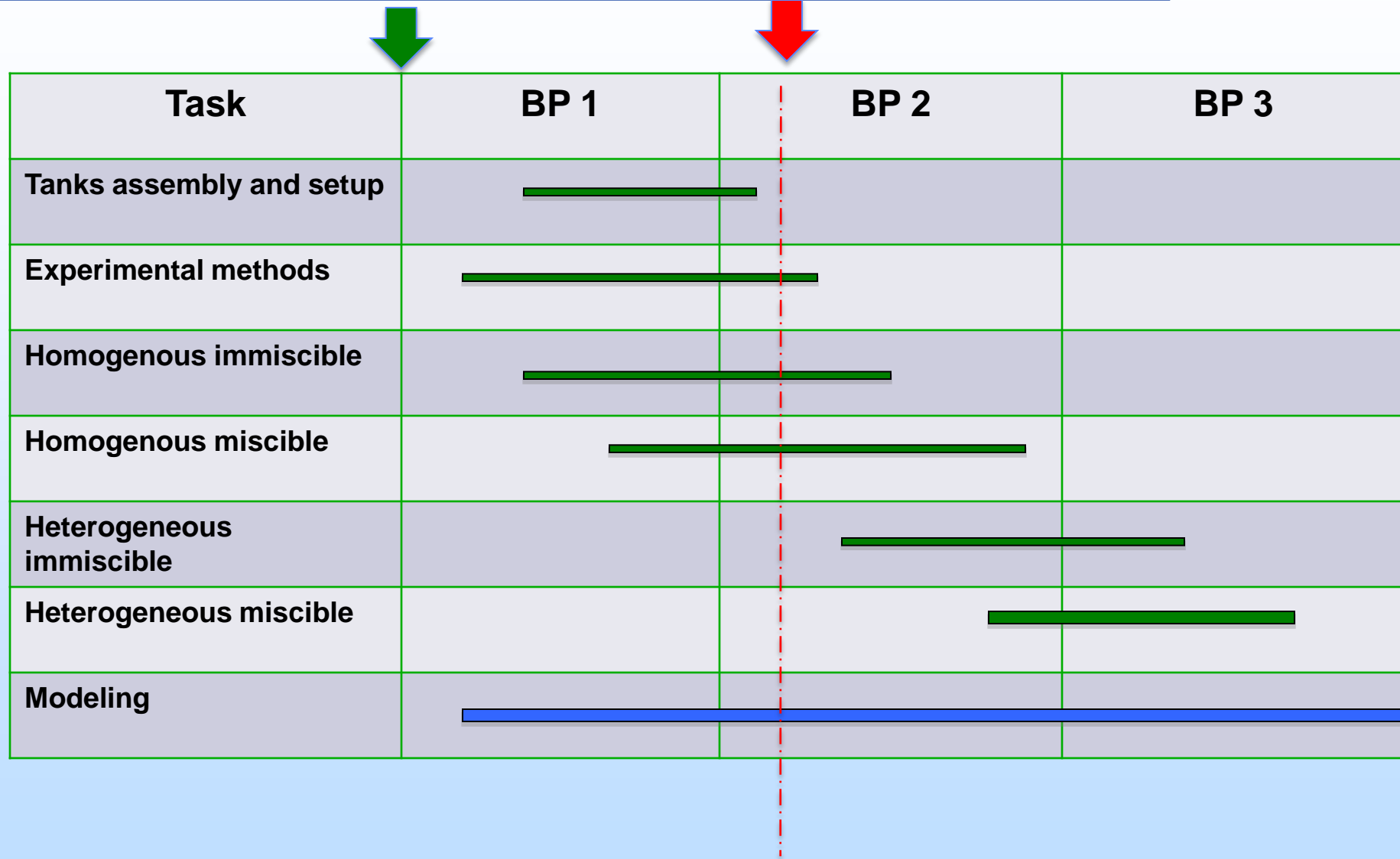
Appendix: Organization and Gantt Charts



Task 1.0 – Project Management and Planning



Updated Time Line



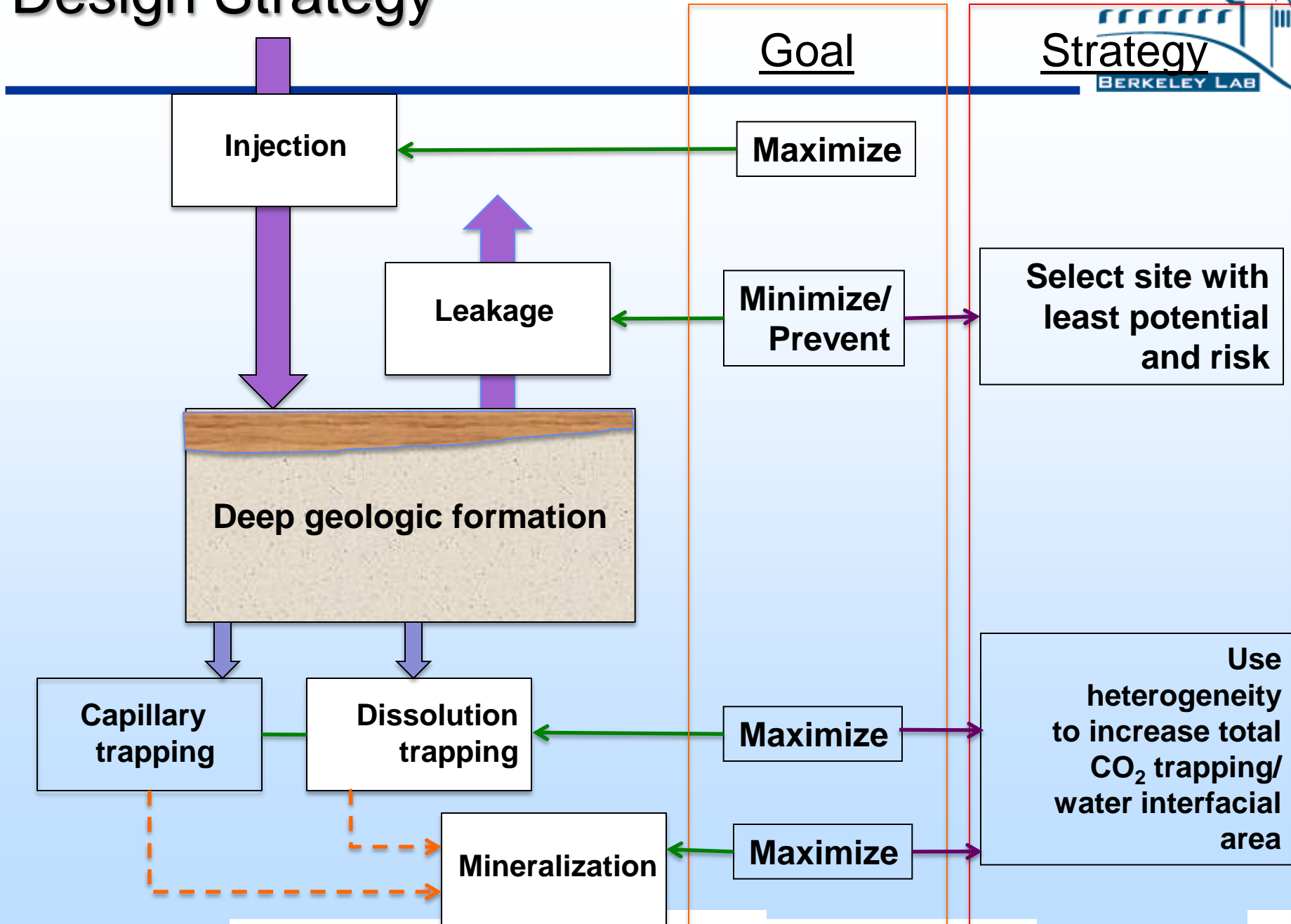
Appendix: Bibliography



Backup Slides



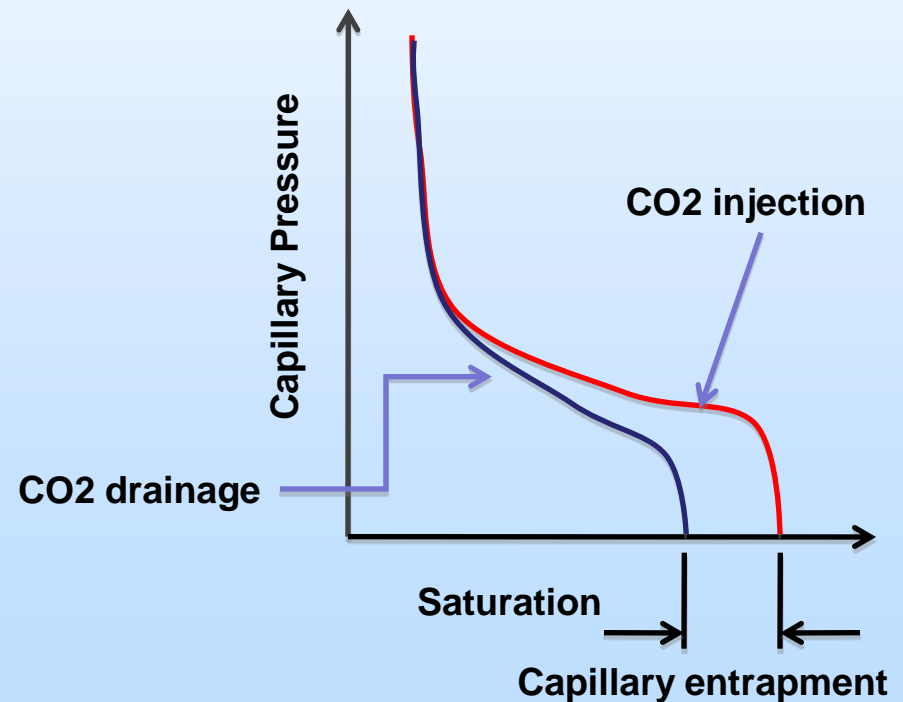
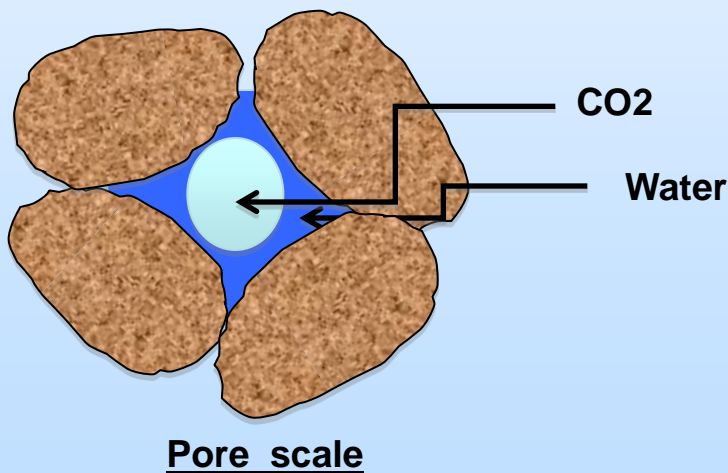
Design Strategy



Physically based theory for predicting entrapment

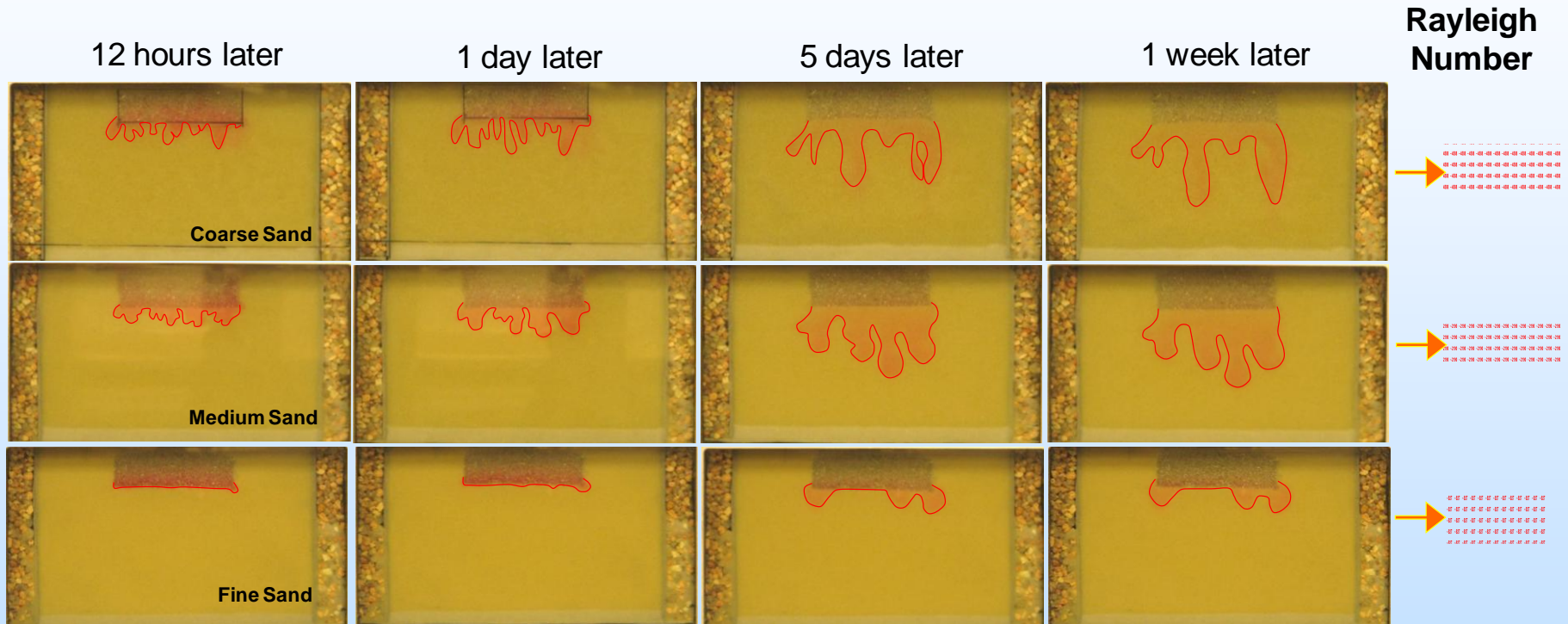
In conventional multiphase flow modeling approaches, **residual non-wetting phase content** are either calculated based on empirical relationships or fitted from experimental data.

There is no physically based theory predicting entrapment of CO₂ in homogeneous and heterogeneous systems.



Small Tank Experiments: Density-driven fingering and (water/propylene glycol) in homogeneous domains

Rayleigh Number for scCO₂-brine @ Typical Reservoir Conditions ~ 6 - 10³

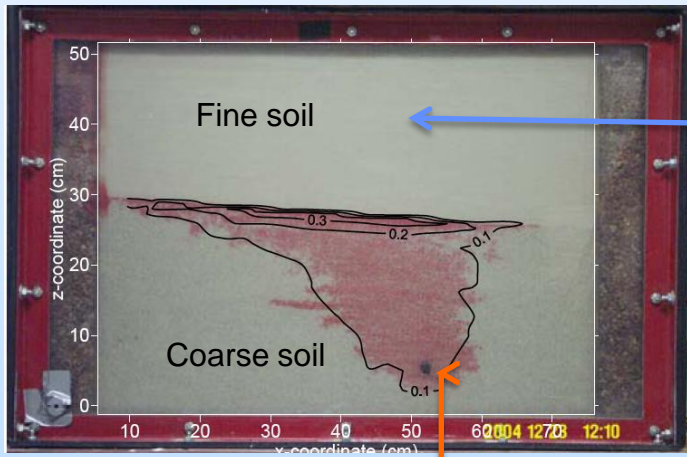


$$Ra = \frac{k\Delta\rho gH}{D\mu\phi}$$
$$Ra_c > 4\pi^2 (\sim 40)$$

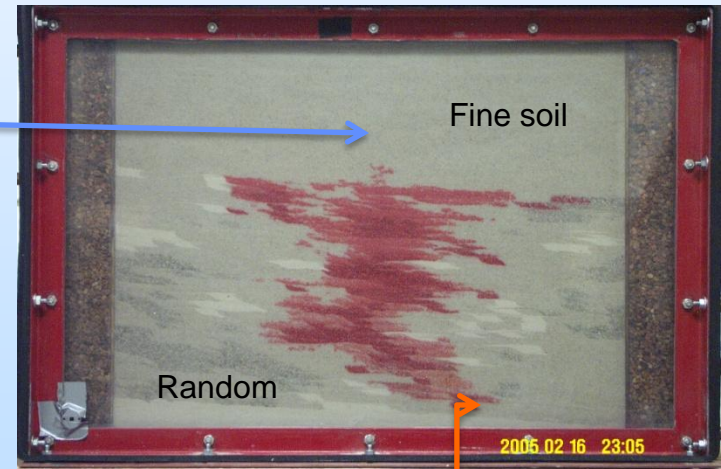
Heterogeneity and Capillary Trapping

Entrapment efficiencies of CO_2 (*defined as the total mass trapping per unit volume of the formation*) in relatively homogeneous and highly heterogeneous systems can be quite different. Knowledge gaps exist on how the heterogeneity influences capillary entrapment of CO_2 .

Homogeneous



Heterogeneous

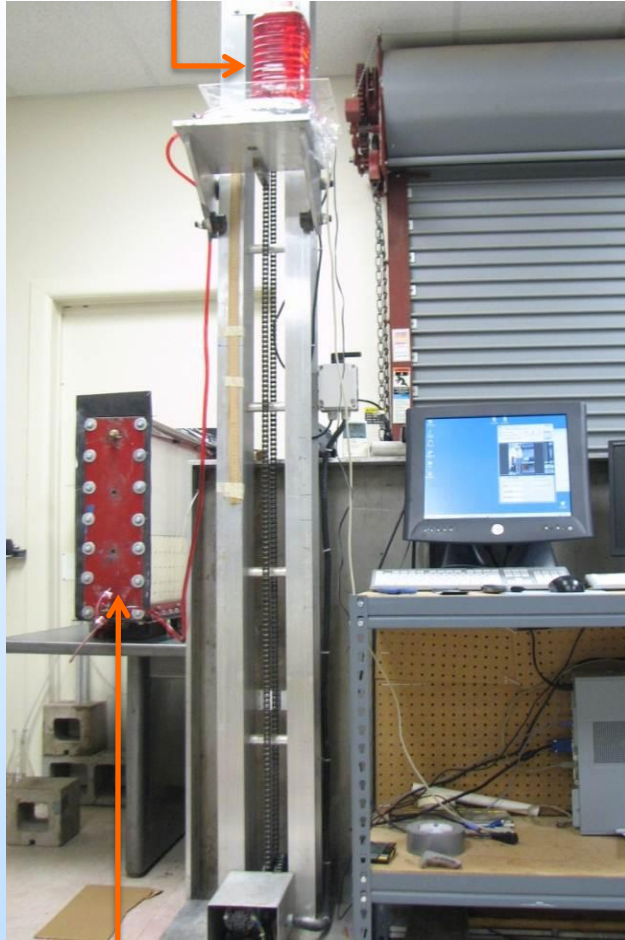


Cap rock

Injection

Small Tank Experiments for Capillary Trapping

Mariotte bottle with Soltrol 220
on an automated balance



Small tank (90 cm x 60 cm x 5.6 cm)

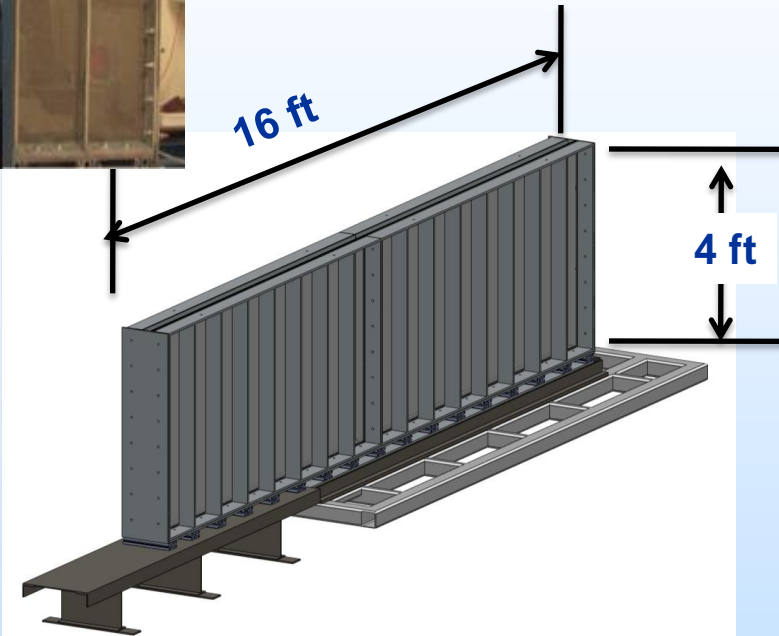
Goal is to generate a data set for validation of models to simulate macro-scale processes of capillary entrapment

- ❑ A total of 8 small tanks experiments with both homogeneous and heterogeneous packing completed.
- ❑ Plume injection and plume configuration recorded.
- ❑ Soil samples removed and the fluids extracted to determine final entrapment saturations.

Large Tank Experiments: Design and assembly of large tanks for confined conditions



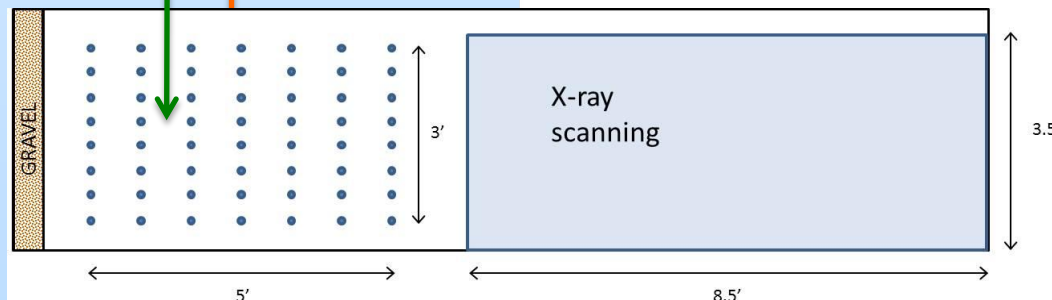
Sloping capping layer



X-ray attenuation
For phase saturation
measurement



Ports for aqueous
sampling

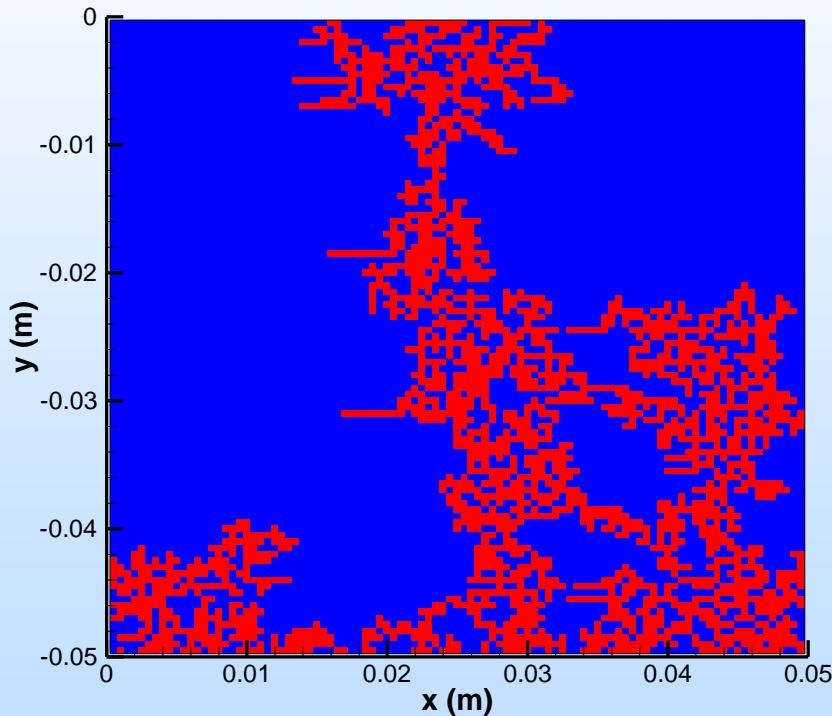


Conceptual Model : Near-Pore-Scale Macroscopic Invasion Percolation

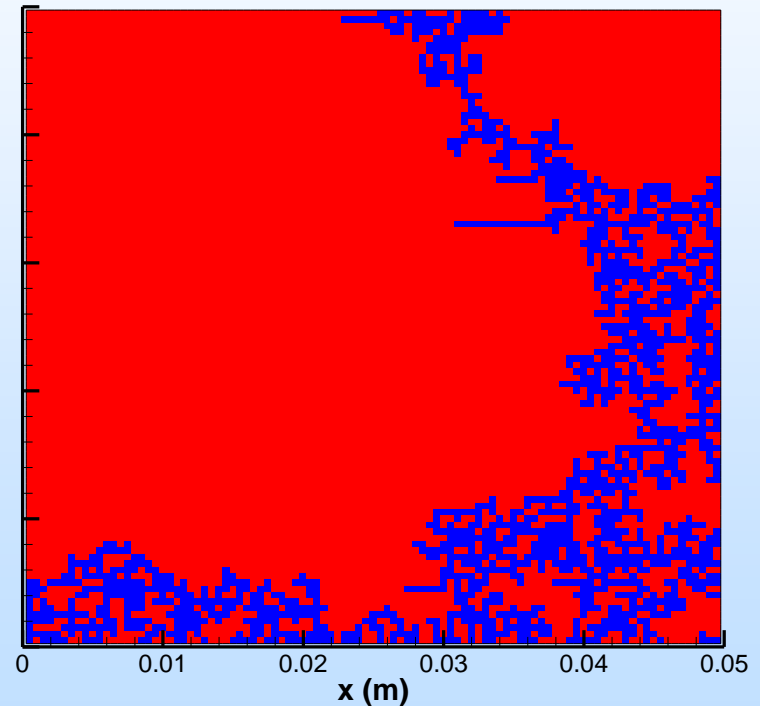


- ❑ Problem domain discretized into a grid (two- or three-dimensional) with a chosen critical “throat” or critical “pore”, r_m , values assigned to each grid block for nonwetting or wetting fluid invasion (Glass et al., 2001, WRR)
- ❑ A grid block contains a small void space characterized with a r_m value.

No Trapping $Young - Laplace Equation, P_c = P_a - P_w = \frac{2\sigma}{r_m}$



Drainage path



Imbibitions path

Development of Constitutive Models Using Pore Connectivity

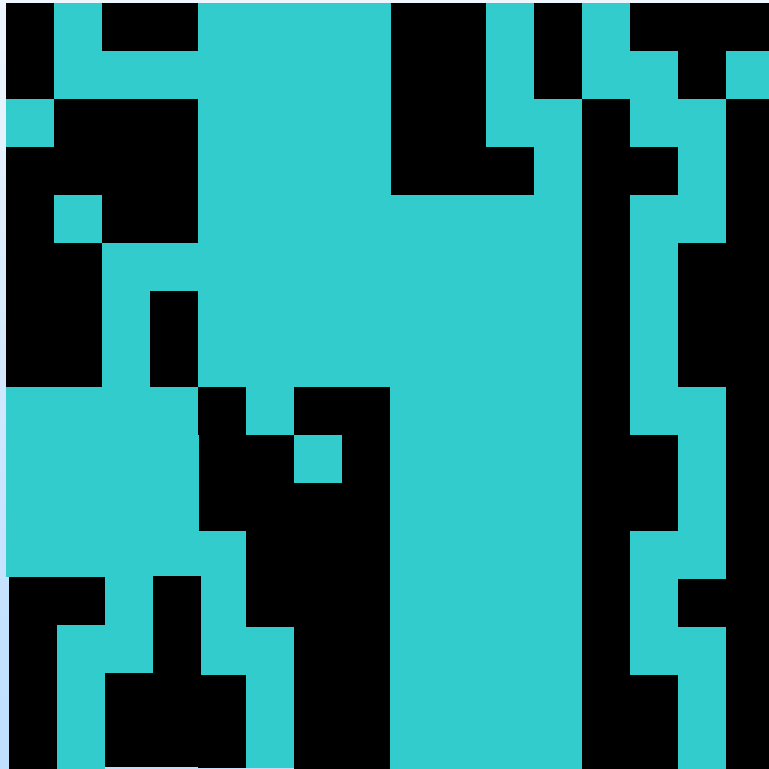


$$\text{Young - Laplace Equation, } P_c = P_a - P_w = \frac{2\sigma}{r_m}$$

Assumptions:

- During drainage, the largest pores drain first
- During wetting, the smallest pores fill up first

Drainage



$$i = 1 \quad \phi - \theta_1 = p_{11}f_1$$

$$i = 2 \quad \theta_1 - \theta_2 = p_{12}(1 - p_{11})f_1 + p_{22}f_2$$

$$p_{11} = 5/6$$

$$p_{12} = 1, \quad p_{22} = 54/60$$

Development of A Theoretical Hysteresis Model



Pore Sizes $r_1 > r_2 > \dots > r_n$

Volume Fractions f_1, f_2, \dots, f_n

Connectivity for the Drainage Paths

Large Pores

$$\begin{array}{cccc}
 p_{11}^d & & & \\
 p_{12}^d & p_{22}^d & & \\
 p_{13}^d & p_{23}^d & p_{33}^d & \\
 \vdots & \vdots & \vdots & \ddots \\
 p_{1n}^d & p_{2n}^d & p_{3n}^d & \dots
 \end{array}$$

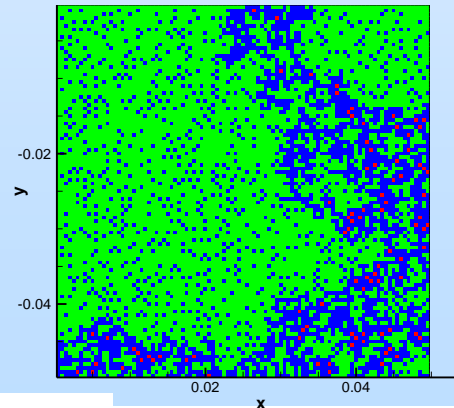
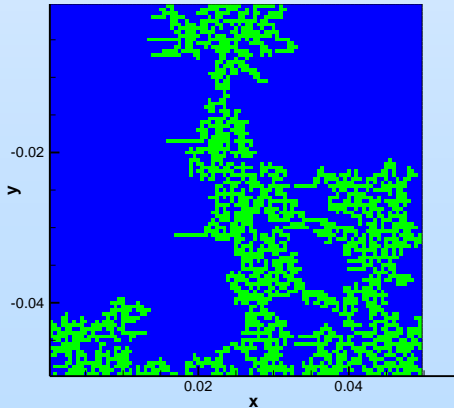
Small Pores

Connectivity for the Imbibitions Paths

$$\begin{array}{cccc}
 p_{n,n}^w & & & \\
 p_{n,n-1}^w & p_{n-1,n-1}^w & & \\
 p_{n,n-2}^w & p_{n-1,n-2}^w & p_{n-2,n-2}^w & \\
 \vdots & \vdots & \vdots & \ddots \\
 p_{n,1}^w & p_{n-1,1}^w & p_{n-2,1}^w & \dots
 \end{array}$$

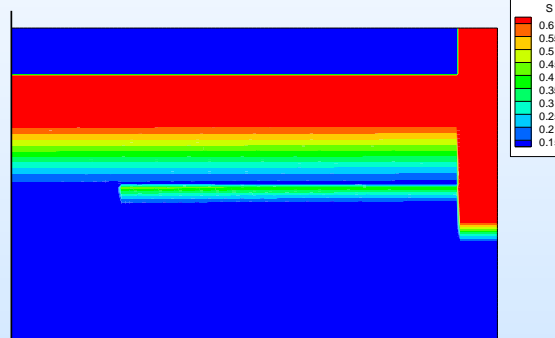
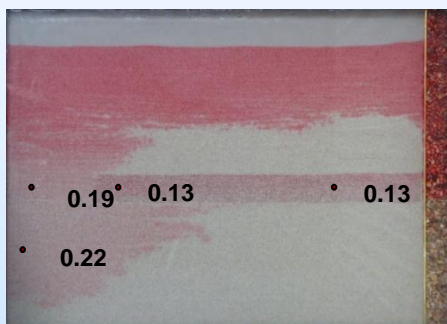
Small Pores

Large Pores

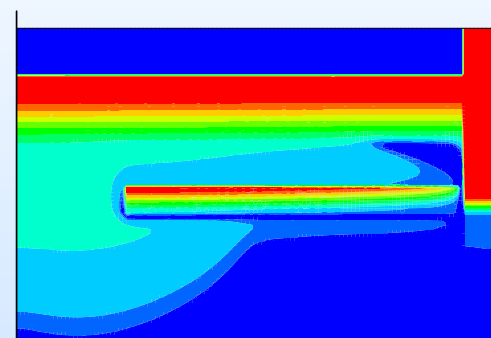


A Small Tank Experiment – Post-Injection

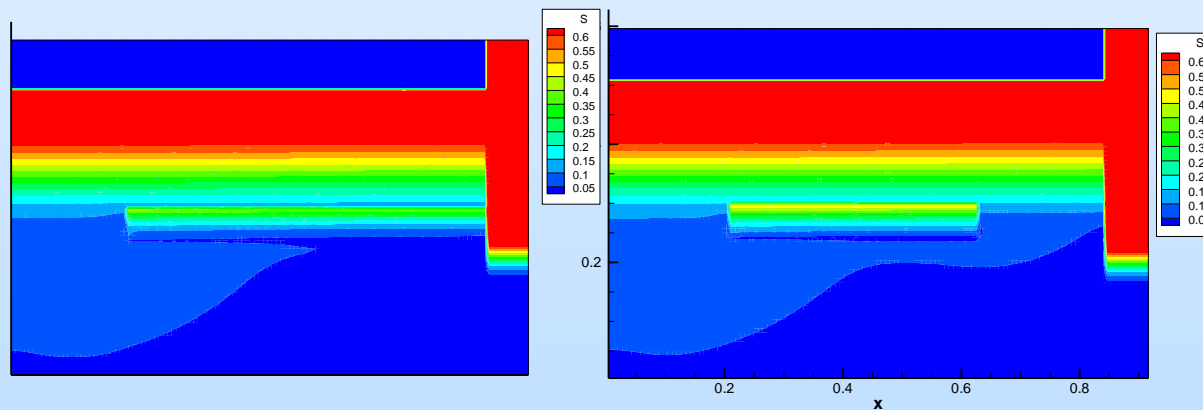
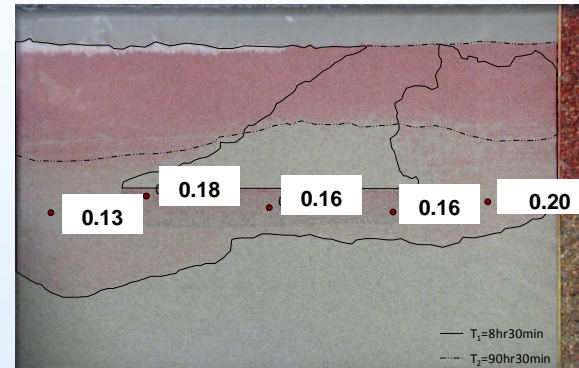
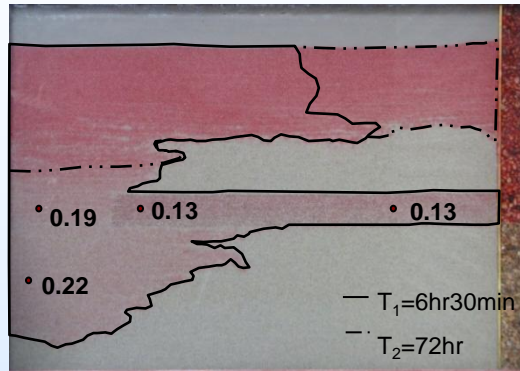
No hysteresis effects



With hysteresis



Saturation distributions at the end of the experiments Heterogeneous Packings

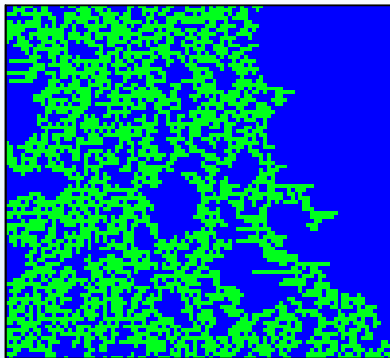


Two-phase model results with hysteresis effects

Dependence of Residual Saturation on Maximum Saturation

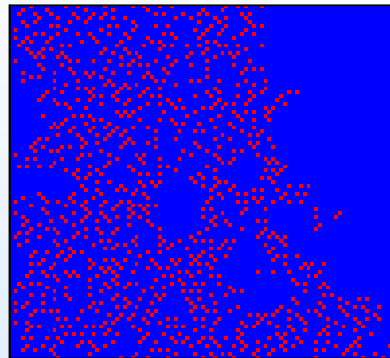
Near-Pore Scale Invasion Percolation (sand#30)

End of Drainage

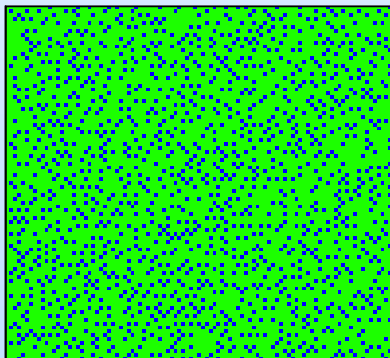


$S_{\max}=0.40$

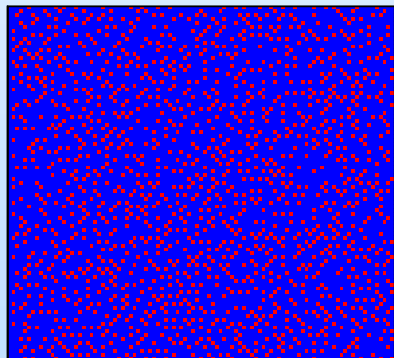
End of Imbibitions






$S_r=0.11$



$S_{\max}=0.84$



$S_r=0.17$

-  Wetting Phase
-  Non-wetting Phase
-  Trapped Non-wetting Phase

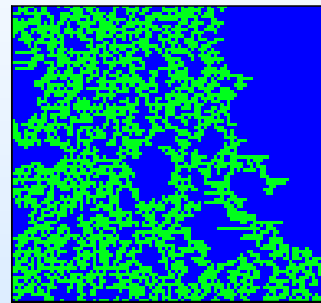
Dependence of Residual Saturation on Maximum Saturation

Results show that the residual non-wetting phase saturation is strongly function of the saturation at the end of injection

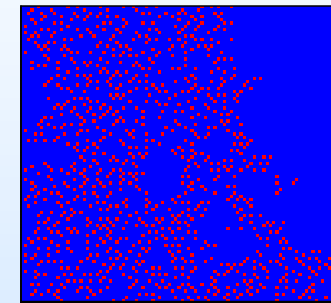
Near-Pore Scale Invasion Percolation (sand#30)

End of Drainage

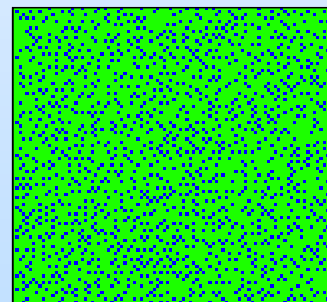
End of Imbibitions



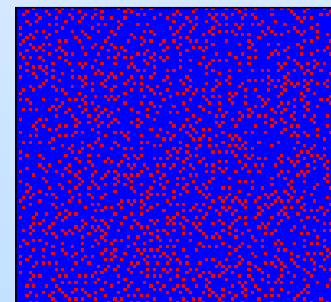
$S_{max}=0.40$



$S_r=0.11$



$S_{max}=0.84$



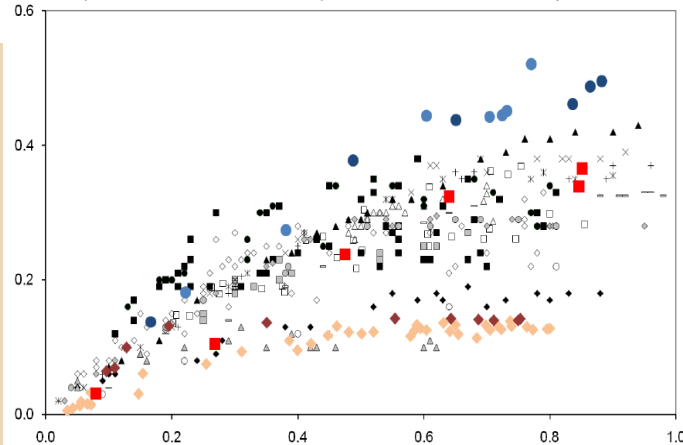
$S_r=0.17$

■ Wetting Phase
■ Non-wetting Phase
■ Trapped Non-wetting Phase

Pentland et al. 2010, SPE

- Crowell et al., 1966
- Kleppe et al., 1997
- ▲ Land (Alundum), 1971
- ◆ Suzanne et al., 2003 ($\phi < 0.085$)
- × Suzanne et al., 2003 ($\phi = 0.13$)
- Suzanne et al., 2003 ($\phi = 0.19$)
- Results of this study - ETP oil/water Berea
- △ Geffen et al., 1952
- Kralik et al., 2000
- Ma & Youngren, 1994
- ◇ Suzanne et al., 2003 ($\phi = 0.10$)
- × Suzanne et al., 2003 ($\phi = 0.15$)
- ◆ Results of this study - oil/water sandpack
- Results of this study - ETP oil/water Clashach
- Jerauld, 1997
- ▲ Land (Berea), 1971
- Pickell et al., 1966
- ◇ Suzanne et al., 2003 ($\phi = 0.12$)
- Suzanne et al., 2003 ($\phi = 0.17$)
- Results of this study - gas/water sandpack
- Results of this study - ETP CO2/water Berea

Residual saturation



Non-wetting phase saturation (at the end of injection)