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

(DE-FE0004630)

Tissa H. Illangasekare
Center for Experimental Study of Subsurface Environmental Processes (CESEP),
Colorado School of Mines, Golden, CO

U.S. Department of Energy
National Energy Technology Laboratory
Carbon Storage R&D Project Review Meeting
Developing the Technologies and
Infrastructure for CCS
August 20-22, 2013

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

(DE-FE0004630)

Tissa H. Illangasekare, Luca Trevisan, Elif Agartan, Hiroko Mori & Javier Vargas-Johnson
Center for Experimental Study of Subsurface Environmental Processes (CESEP), Colorado School of Mines, Golden, CO

Abdullah Cihan, Jens Birkholzer, Marco Bianchi, Quanlin Zhou
Earth Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA

Presentation Outline

- ☐ **Project Overview** - Goals & Objectives
  - Benefits of technology
  - Project status
- ☐ **Key questions and knowledge gaps**
  - Successful storage
  - Role of models in design
  - Conceptualization and key questions
- ☐ **Objectives and tasks**
- ☐ **Multi-scale physical and numerical modeling approach**
  - Experimental methods
- ☐ **Technical progress and results**
  - Experimental results
  - Modeling results
- ☐ **Findings**
- ☐ **Future Plans**
- ☐ **Appendix**

Benefits of Technology to the Program

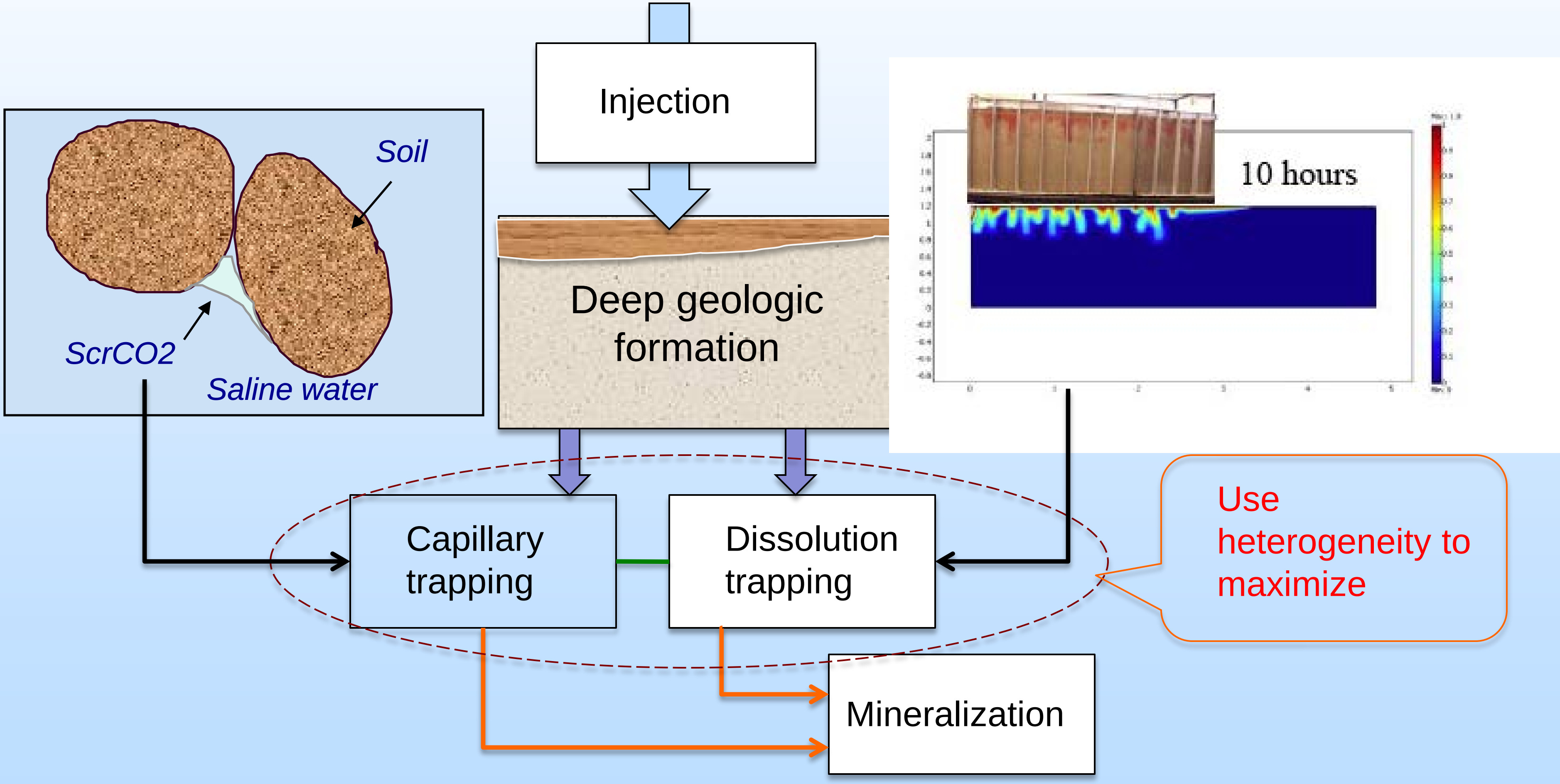
- ☐ Improve/develop and validate models by using the data generated in intermediate-scale laboratory test systems (~1 - 5m length) simulating capillary and dissolution trapping under various heterogeneous conditions.
- ☐ Design injection strategies, estimate storage capacities and efficiency for field-scale 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.

Project Overview:
Goals and Objectives

- ☐ Objectives
  - Investigate how the trapping mechanisms are affected by formation heterogeneity with the ultimate goal of contributing towards improving numerical tools and up-scaling methods to design injection strategies, estimate storage capacities and efficiency, and conduct performance assessment for stable storage.
- ☐ Goals
  - The mechanisms of capillary and dissolution trapping that are affected by heterogeneity will be investigated using intermediate scale testing in porous media tanks.
  - The generated data will be used to improve the conceptual understanding and develop and validate models that will allow more accurate prediction of CO2 fate and transport in deep geologic saline formations.

Successful Storage

The goal of successful storage is to create stable conditions where the CO_2 becomes immobilized through entrapment, dissolution, and mineralization.



Injection

Deep geologic formation

Capillary trapping

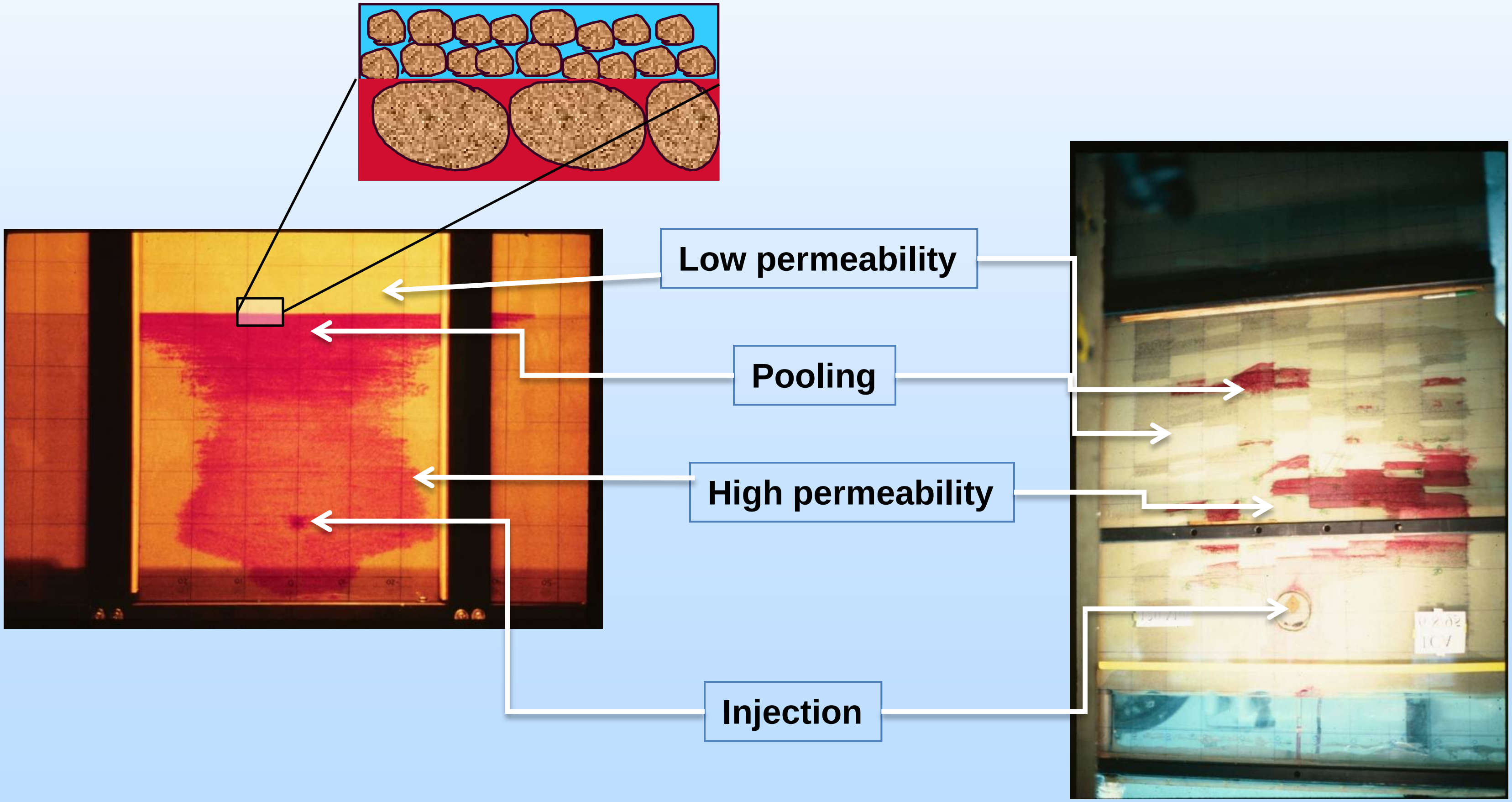
Dissolution trapping

Mineralization

Use heterogeneity to maximize

Conceptualization

In naturally heterogeneous formations, the supercritical CO_2 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 of the non-wetting fluid).



Low permeability

Pooling

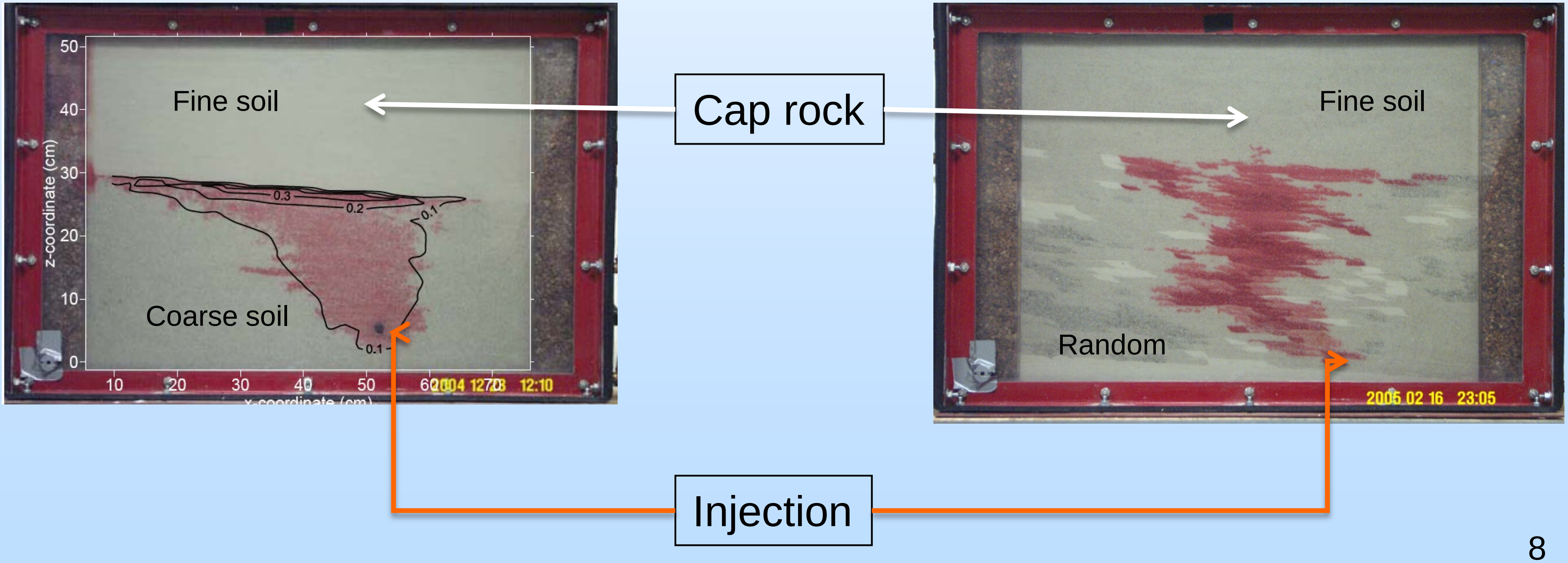
High permeability

Injection

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 ScrCO_2.



Homogeneous

Heterogeneous

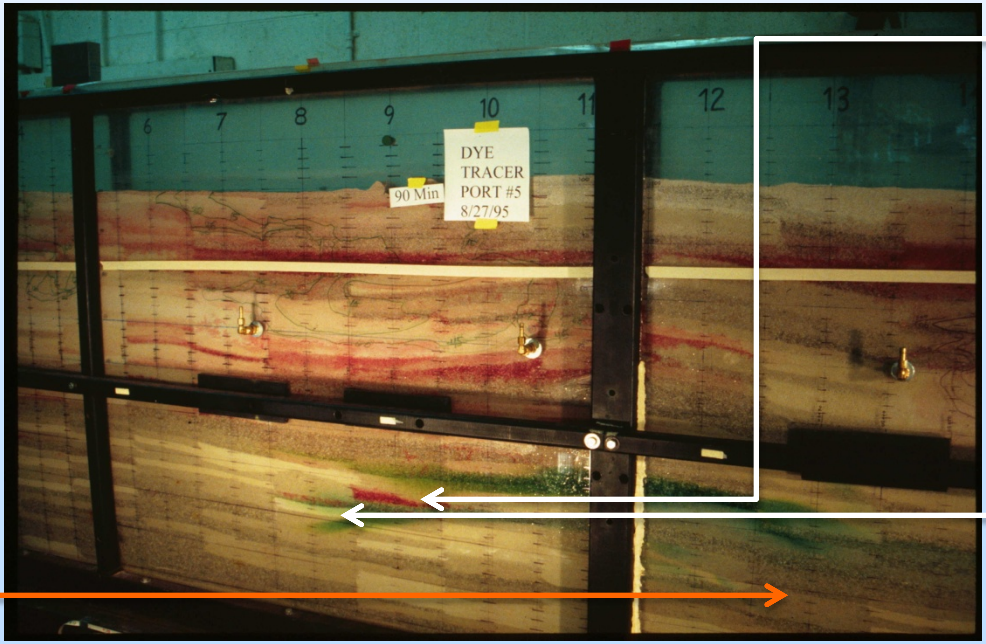
Cap rock

Injection

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.



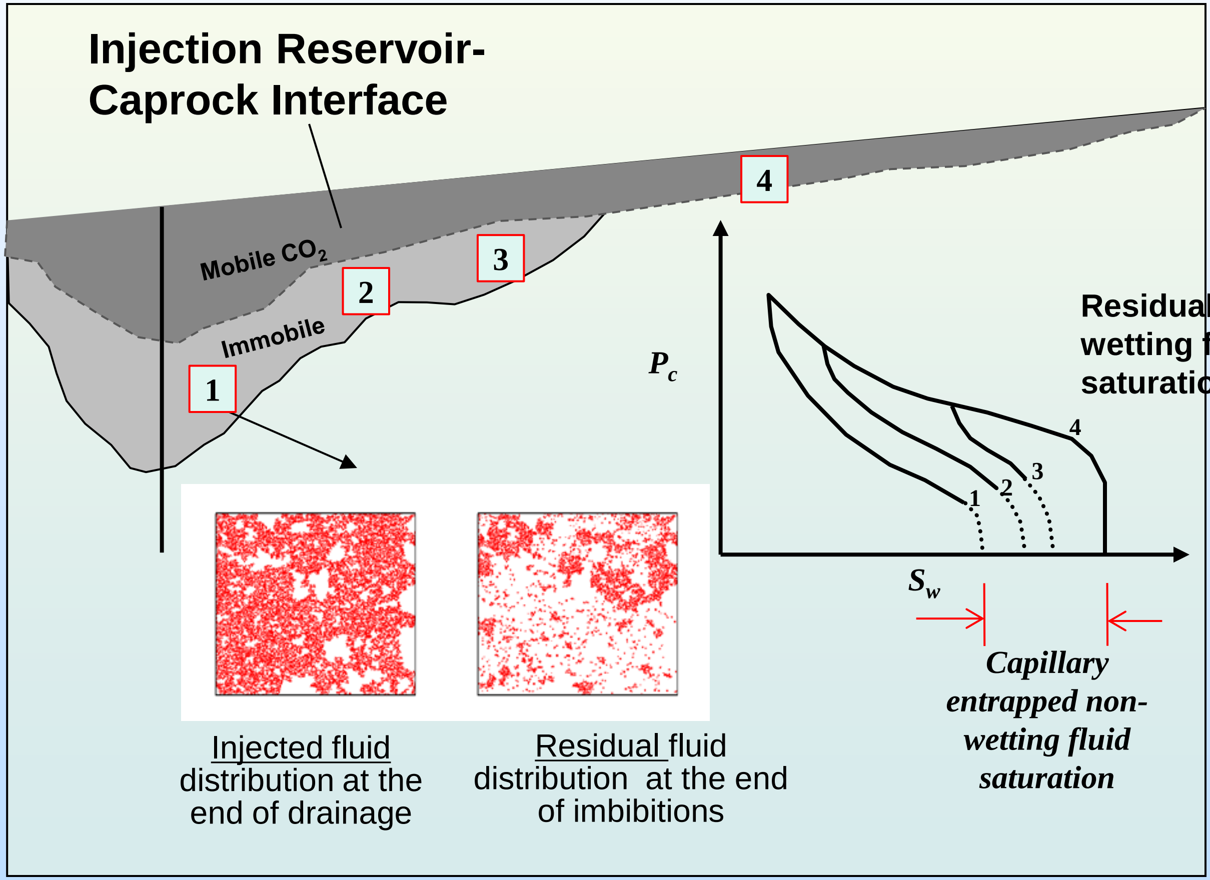
Diffusion into Low-permeability zones

Entrapped ScrCO2

Flowing saline water

Entrapped CO_2 fluid saturation after imbibition is a function of maximum saturation distribution at the end of injection.

Knowledge gap: No physically-based theory exists for representation of hysteresis in constitutive models with capillary trapping at macroscopic scale



Injection Reservoir-Caprock Interface

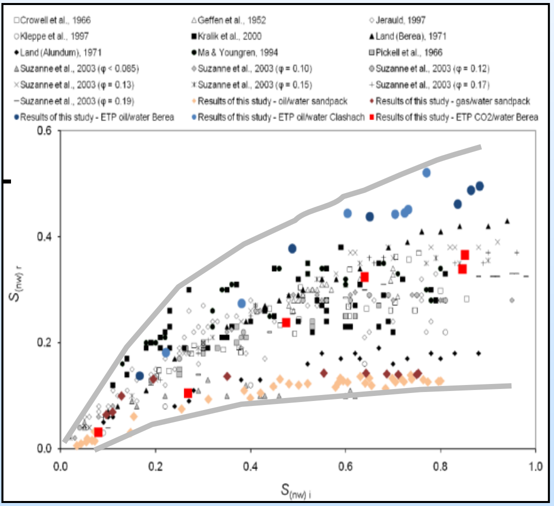
Injected fluid distribution at the end of drainage

Residual fluid distribution at the end of imbibitions

Capillary entrapped non-wetting fluid saturation

Residual non-wetting fluid saturation

Pentland et al. 2010, SPE



Non-wetting fluid saturation at the end of drainage

Research Questions

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 (water/$scCO_2$) flow behavior 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?
- ❑ How effective is diffusion into low permeability zones in enhancing trapping?
- ❑ Under what conditions convective mixing is important?

Project Overview- Scope of Work

- Generate a comprehensive data set in intermediate scale test tanks simulating multiphase flow to investigate how effective capillary trapping at field scale is affected by the texture transitions and variability in heterogeneous field formations.

- Generate a comprehensive data set in intermediate scale test tanks simulating dissolution of partially miscible fluids to investigate how effective dissolution trapping at the field scale is affected by heterogeneity-driven preferential flow and cross-intra-layer mixing.

- Modeling efforts that includes various scenario simulations to evaluate whether the existing modeling codes can accurately capture processes observed in the test tanks. This effort will lead to develop up-scaling methods for larger-scale applications.

Project Overview: Scope of Work

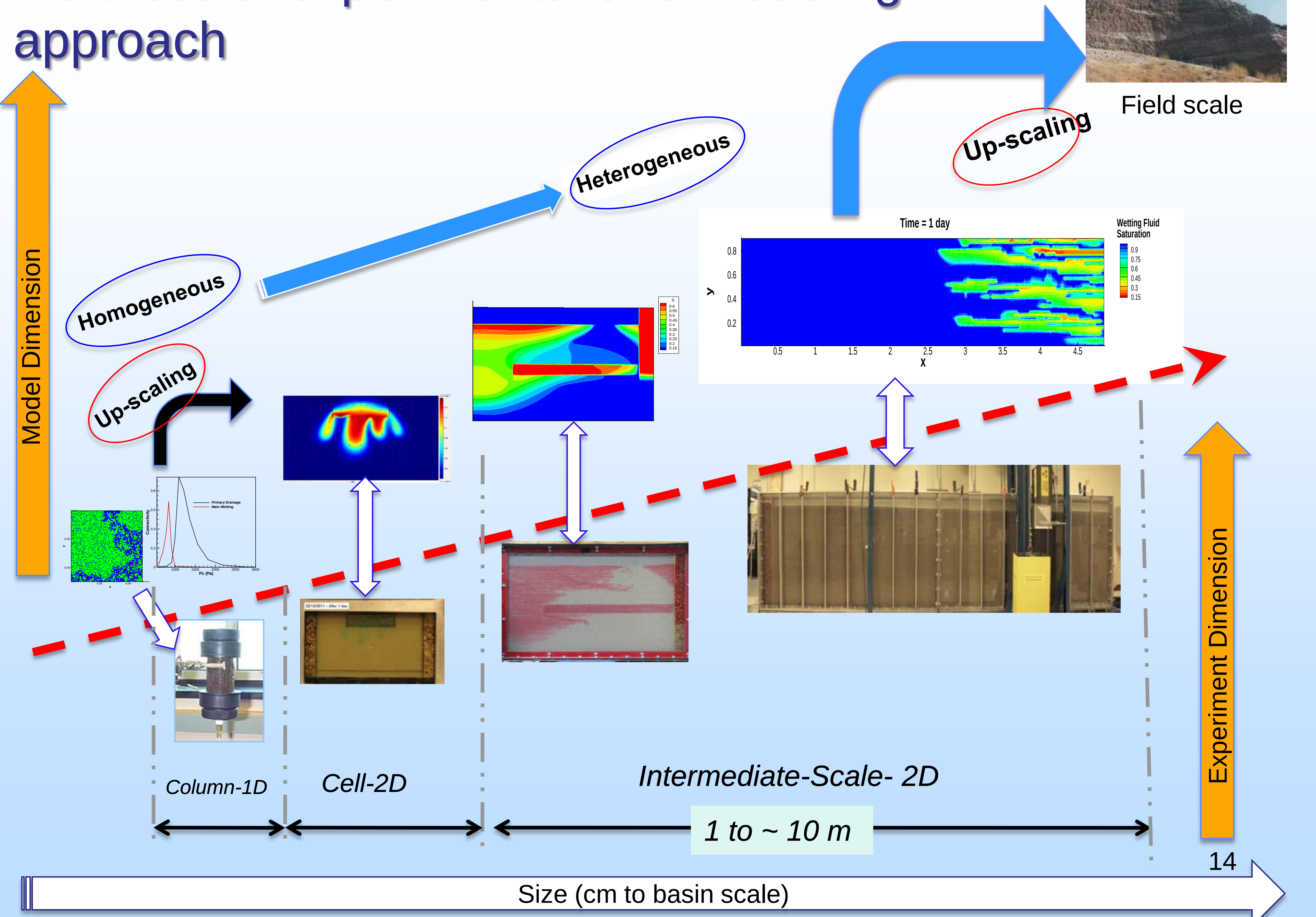
Why has the Scope of Work been defined as it is?

- ☐ Even though trapping at the core-scale is reasonably well understood and empirically modeled for relatively homogenous systems, critical knowledge gaps exist on how these processes manifest themselves under conditions of ubiquitous field heterogeneities to estimate or predict effective trapping capacities of field systems.

- ☐ Comprehensive understanding of the CO2 storage and entrapment problem is only possible through multistage analysis comprising of experimental studies under highly controlled conditions and modeling.

- ☐ To our knowledge, none of the existing modeling tools have been validated or tested for their ability to accurately capture the CO2-brine-water flow patterns and entrapment mechanisms in porous media, specifically under heterogeneous conditions.

Multi-scale experimental and modeling approach



Model Dimension

Homogeneous

Up-scaling

Heterogeneous

Up-scaling

Field scale

Experiment Dimension

Column-1D

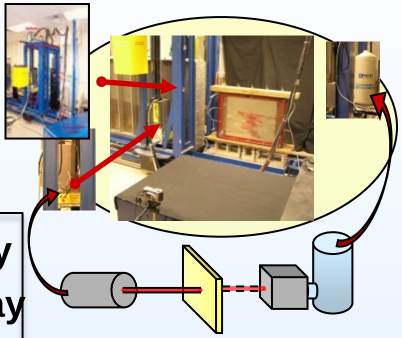
Cell-2D

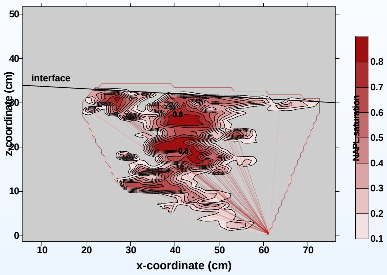
Intermediate-Scale- 2D

1 to ~ 10 m

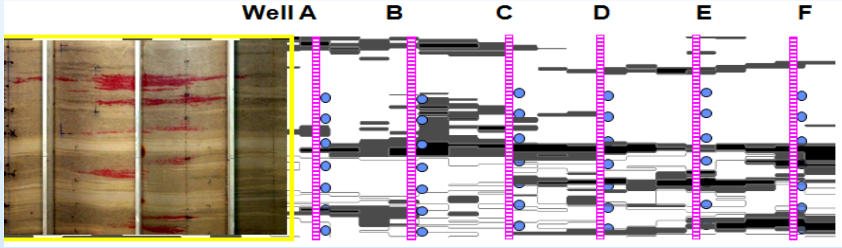
Size (cm to basin scale)

Experimental Methods

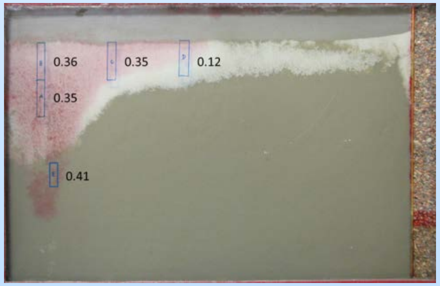




- Automated transient and spatially distributed **saturations** using x-ray attenuation



- 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)

Selection of Surrogate Test Fluids

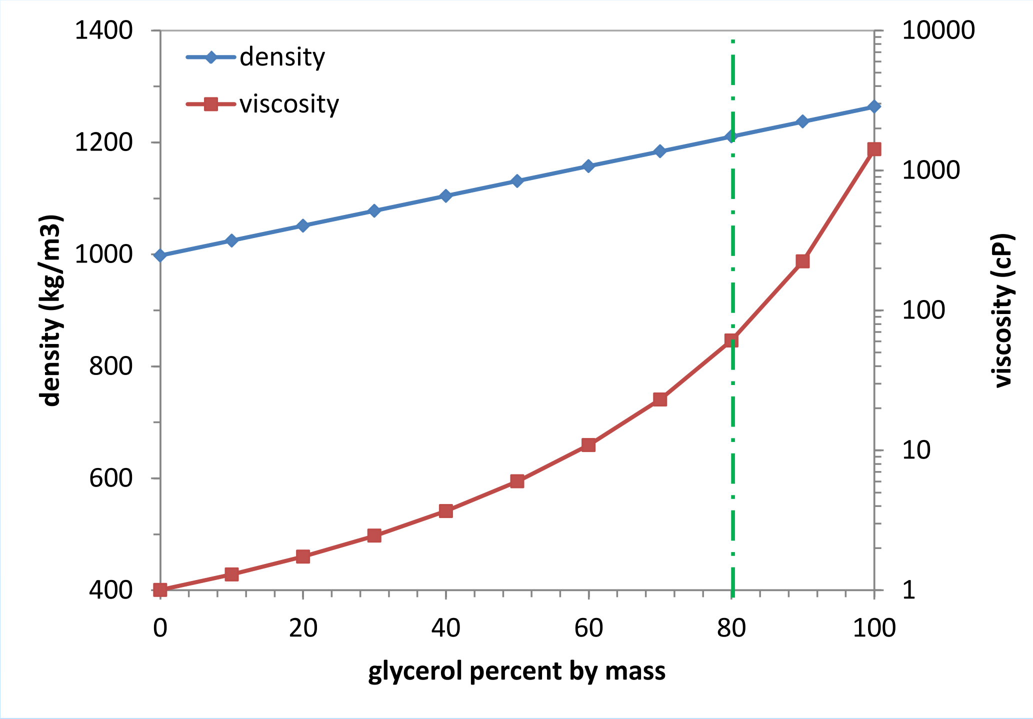
- Laboratory investigation of $scCO_2$ migration without high pressure in deep formations can be conducted using analogous fluids having similar density and viscosity contrasts as $scCO_2$ – brine phases under storage conditions

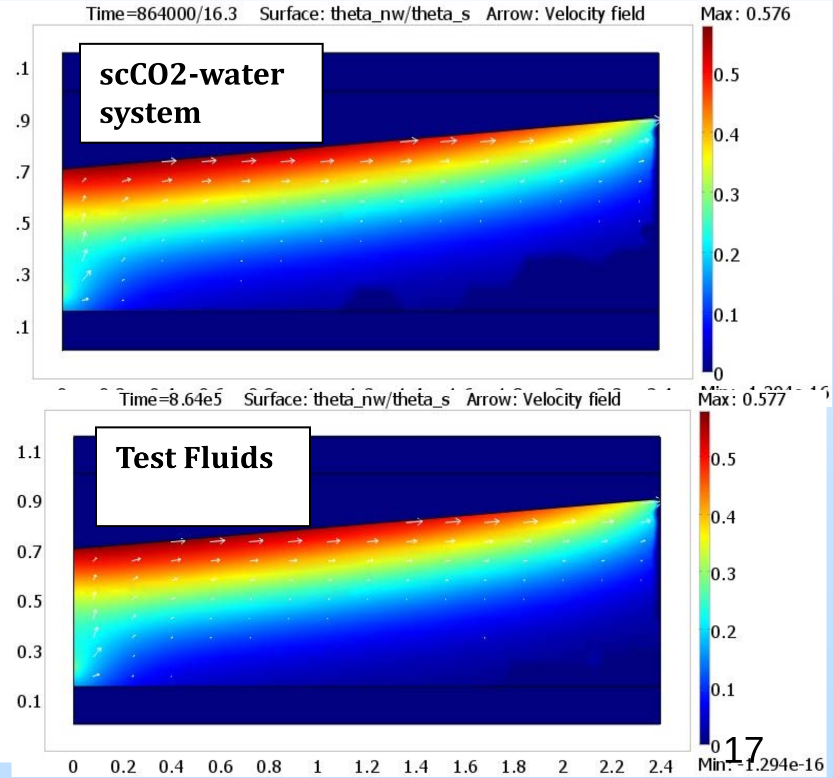
Dimensionless Numbers	scCO2-brine @ Typical Reservoir Conditions	Soltrol220-glycerol/water @ 20C, 1 atm	Water in Propylene Glycol @ 20C, 1 atm	Hexanol in Water @ 20C, 1 atm
Bond # $Bo = \frac{\Delta\rho\, g\, k}{\sigma}$	~ 10^{-7} - 10^{-8}	~10^{-6}- 10^{-7}	~10^{-6}- 10^{-7}	~10^{-6}- 10^{-7}
Capillary # $Ca = \frac{\mu_{nw}\, u_T}{\sigma}$	~ 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	~0.475
Density Ratio $\frac{\rho_{nw}}{\rho_w}$	~ 0.2 – 0.8	~0.66	~0.9	~0.814
Solubility	~3-5 %	immiscible	miscible	0.6%

Numerical Validation of Scaling Approach

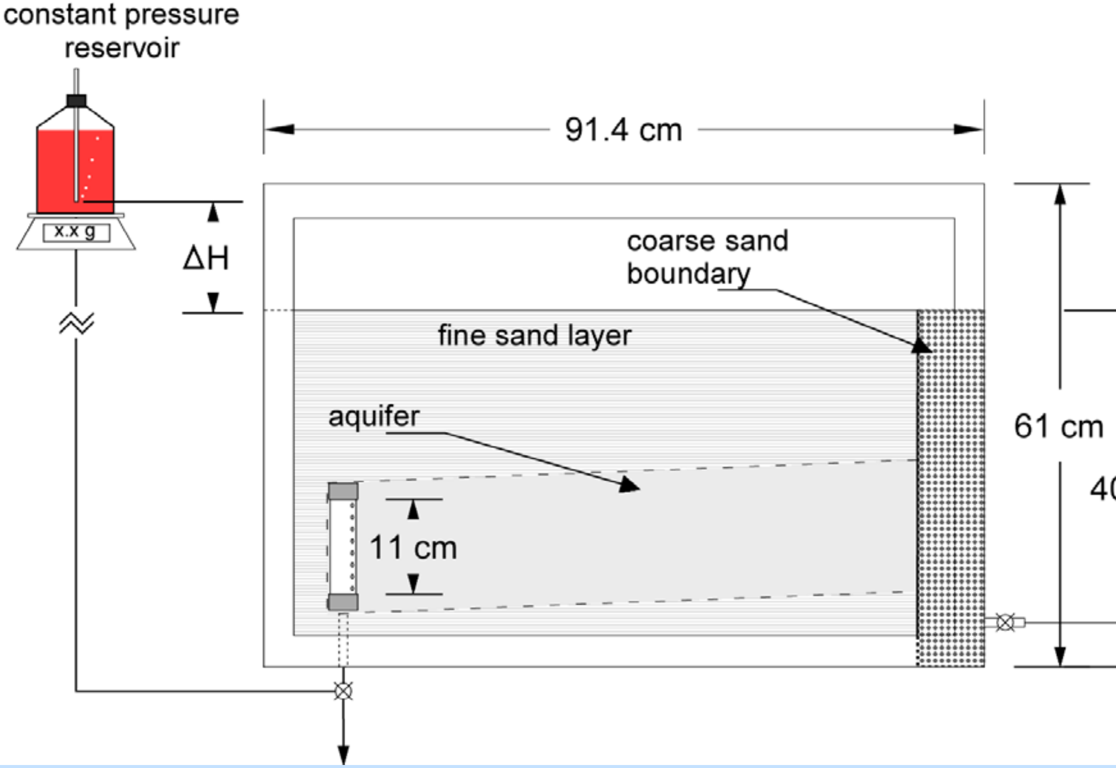
- ☐ Identical results can be obtained if the same dimensionless numbers are chosen for the geometrically similar two systems (Shook et al., 1992; Gharbi et al.,1998).

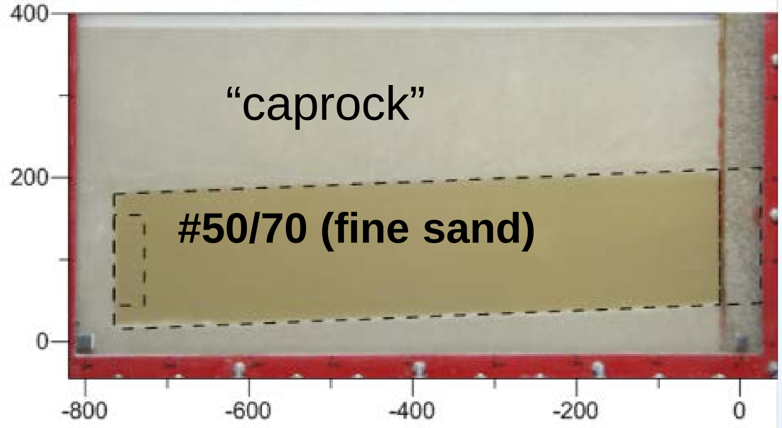
Glycerol/water mixture at ambient conditions

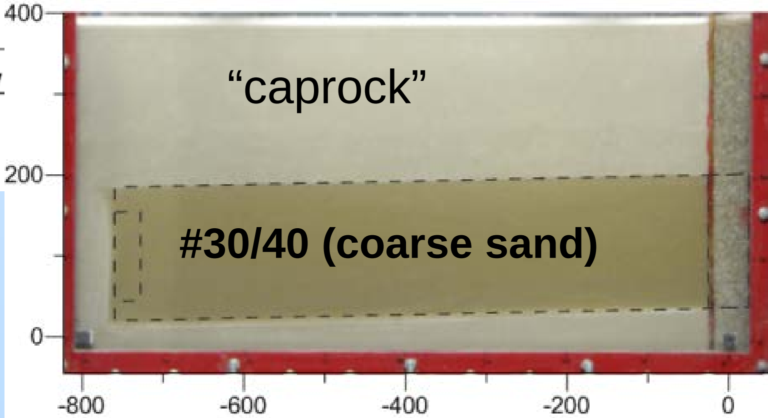




Experiments on trapping in homogeneous systems





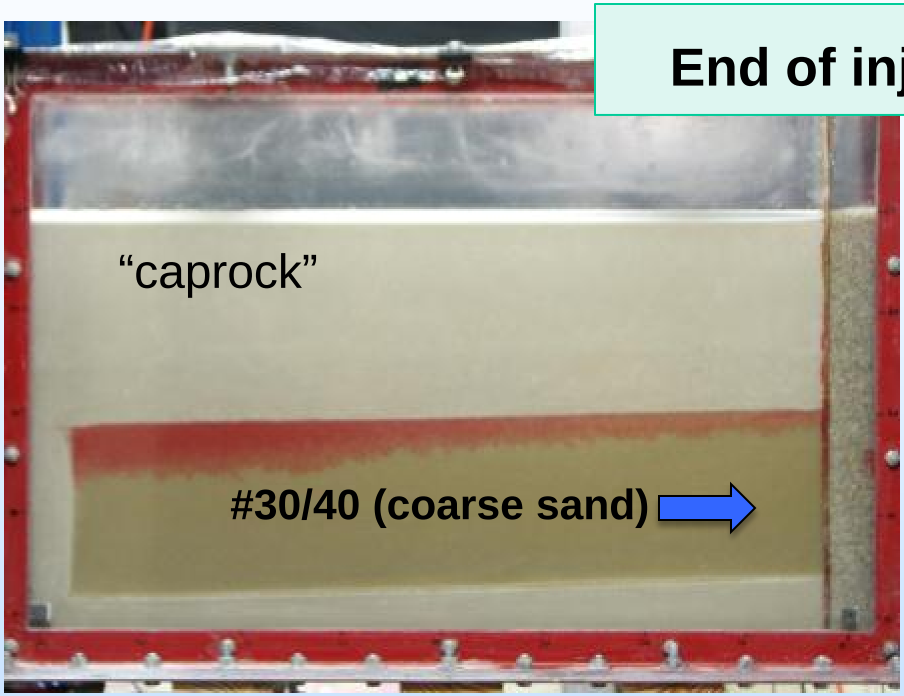


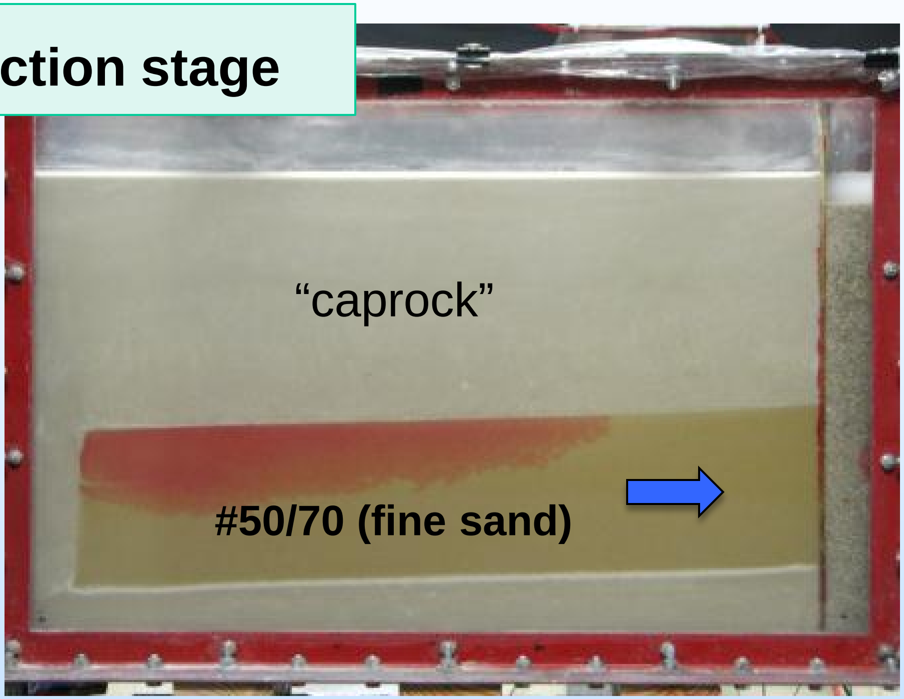
Sweep efficiency related to Bond Number

Max swept volume ~20%

Max swept volume ~30%

End of injection stage





Buoyancy forces ←

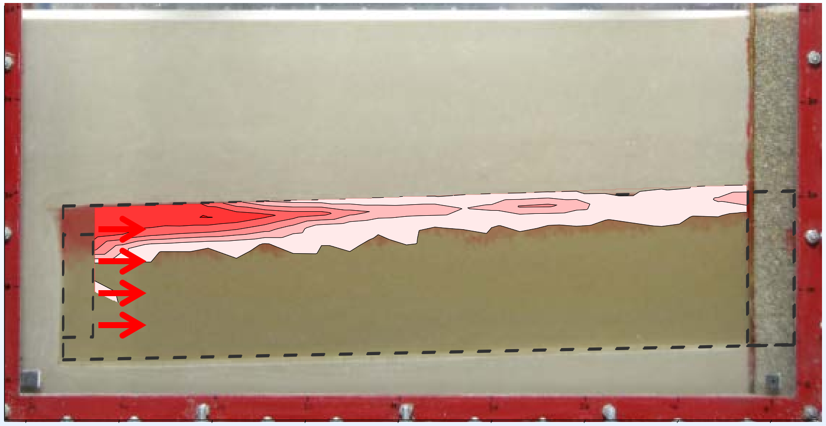
Bo = 5.86E-05

Bo = 9.30E-06

$$Bo = \frac{\Delta\rho\, g\, k}{\sigma}$$

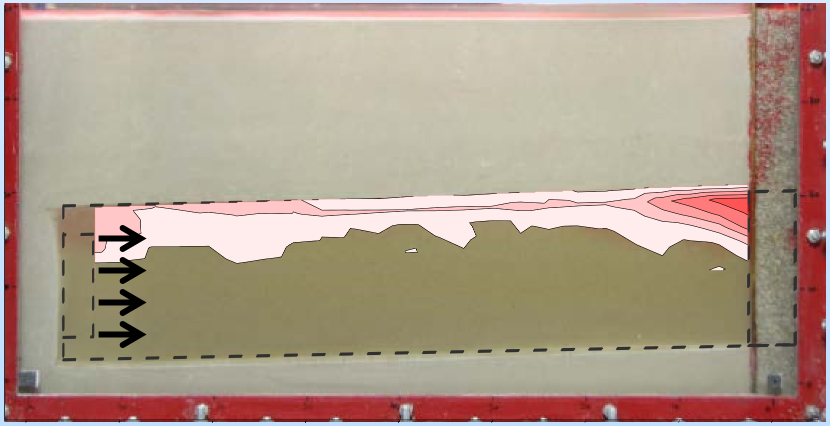
Experiment 1: **#30/40 saturation measurement**

1 hr 47 min



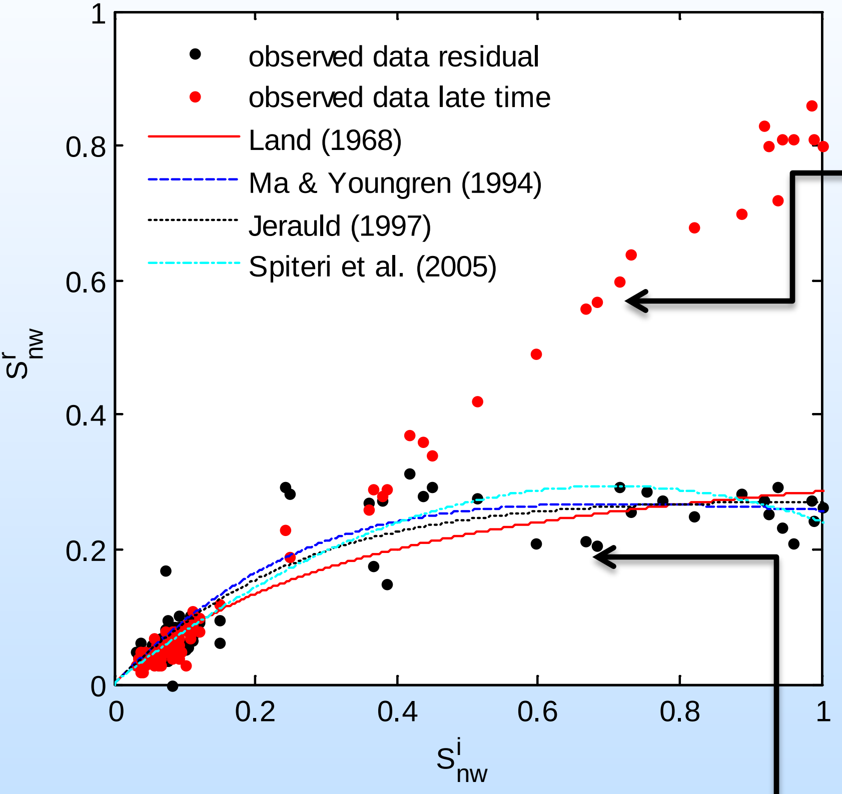
Plume distribution at late time (injection stopped at t = 5hr)

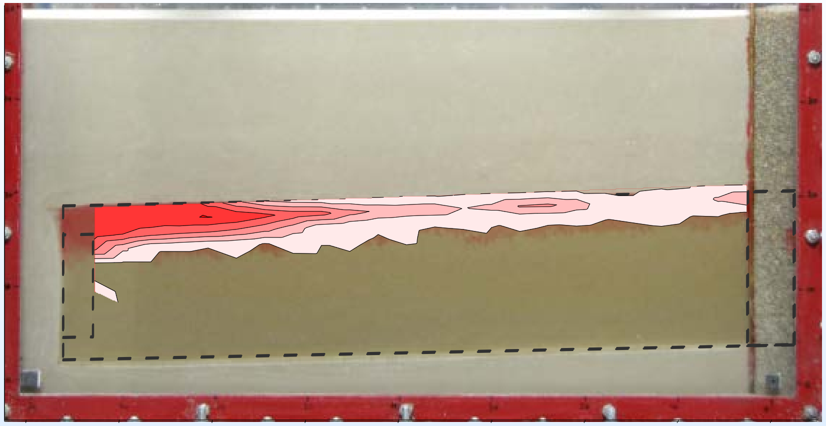
607 hr 46 min

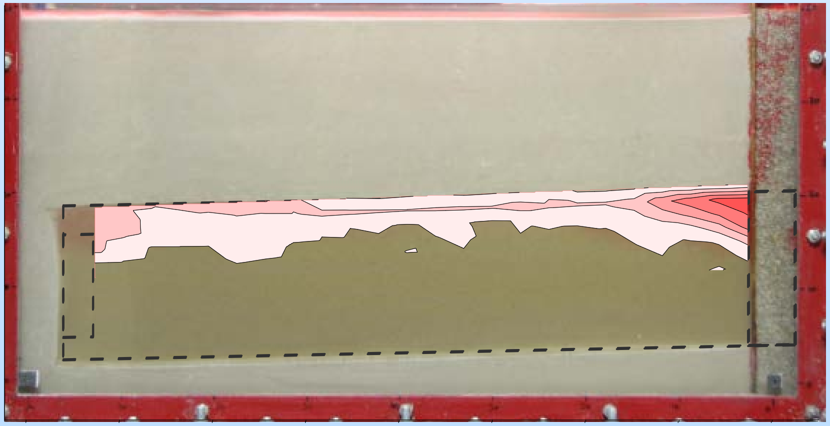


Plume footprint at residual saturation after **sweeping**

Initial-Residual saturation vs final trapping after sweep



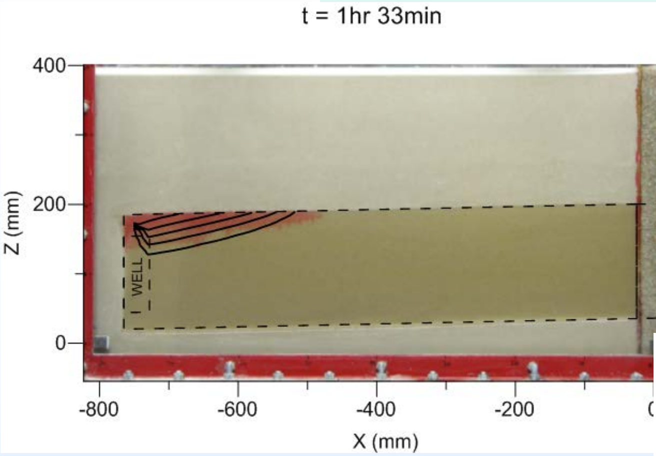


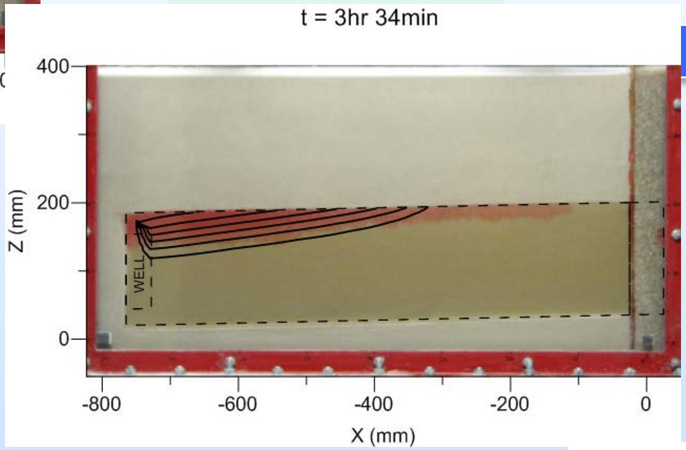


Similar results found by Fagerlund et al., *Vadose Zone Journal*, 2006

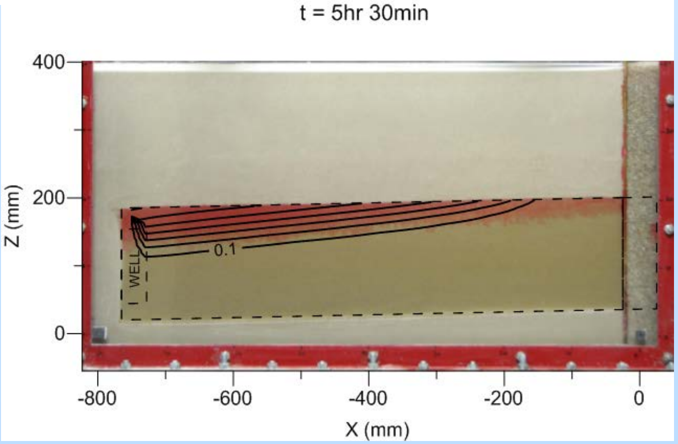
TOUGH2-T2VOC simulations with analog fluids

1 hr 33 min





5 hr 30 min



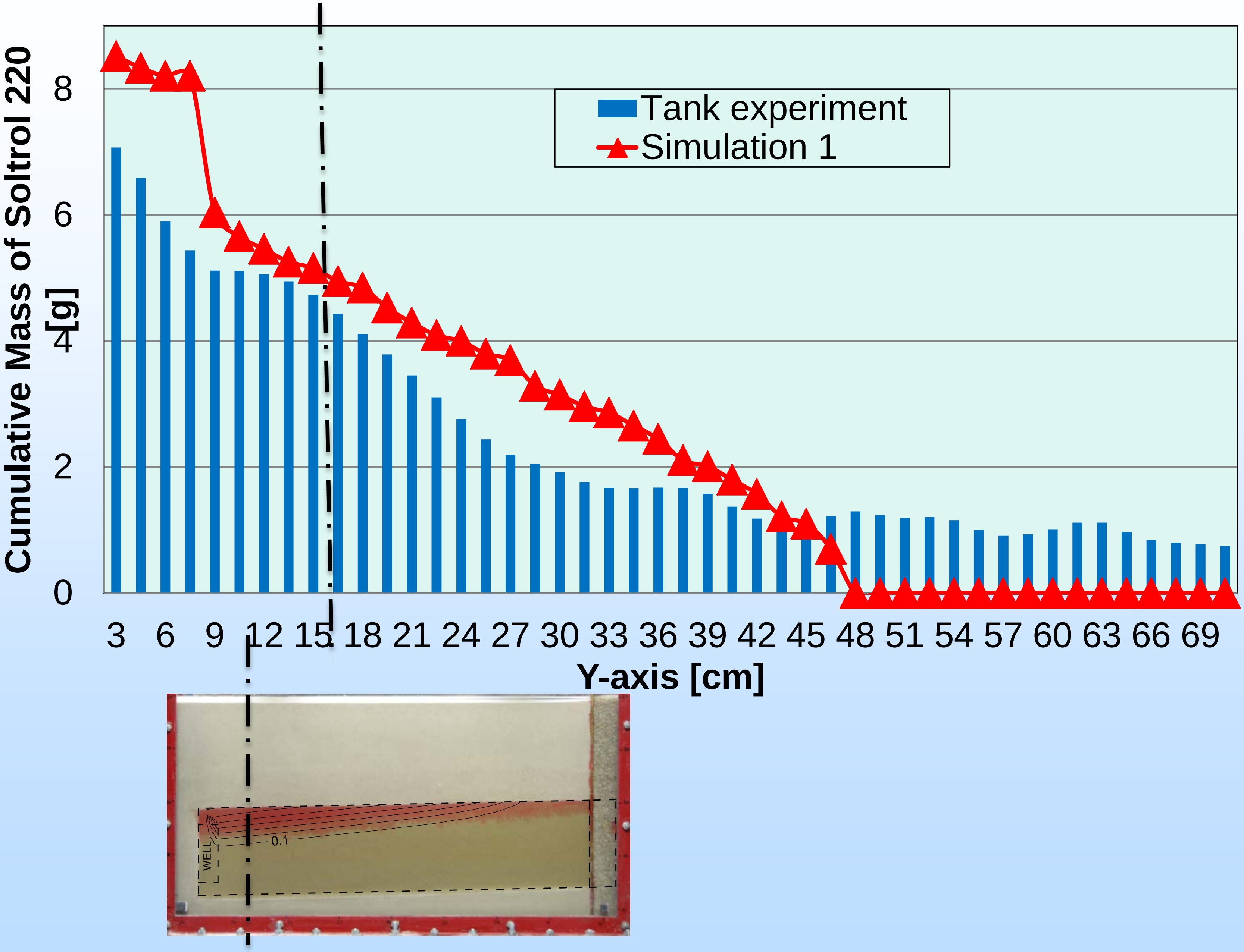
T=20°C, P= 80 kPa

$\rho_{Soltrol}$ = 860 kg/m^3, $\rho_{glycerol/water}$ = 1210 kg/m^3

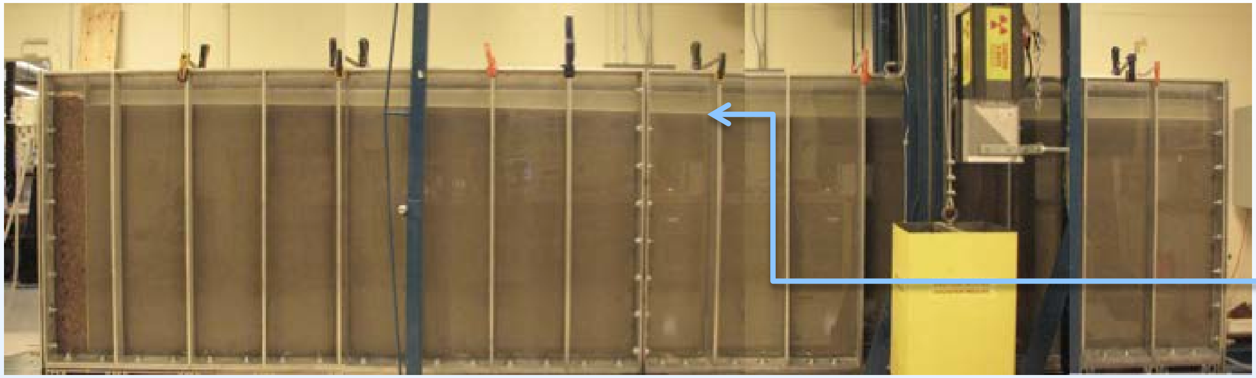
$\mu_{Soltrol}$ = 4.5 mPa·s, $\mu_{glycerol/water}$ = 61 mPa·s

Q = 0.71 ml/min, t = 5.5 h, V_{inj} = 240 ml

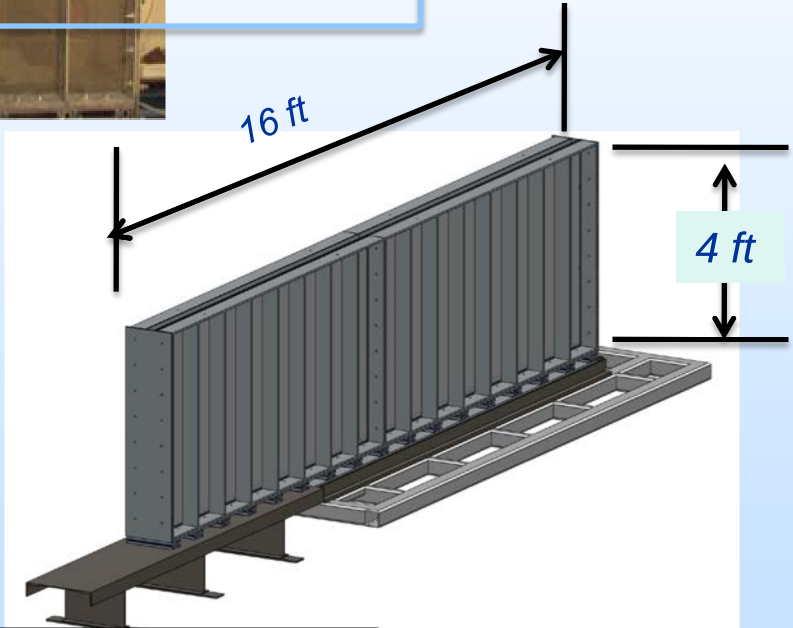
TOUGH2-T2VOC modeling comparison to experiments



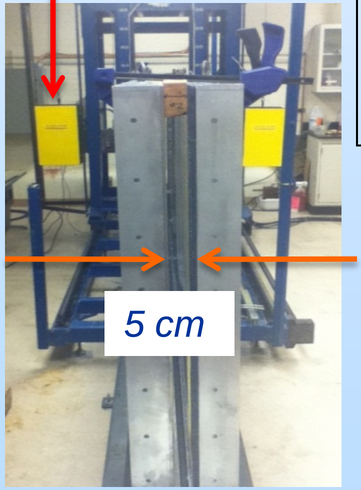
Design and assembly of large tanks



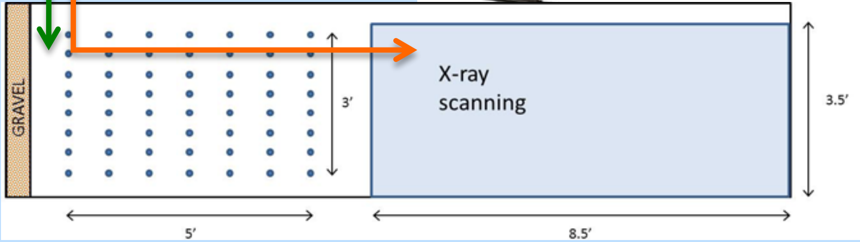
Sloping capping layer



X-ray attenuation
For phase saturation
measurement



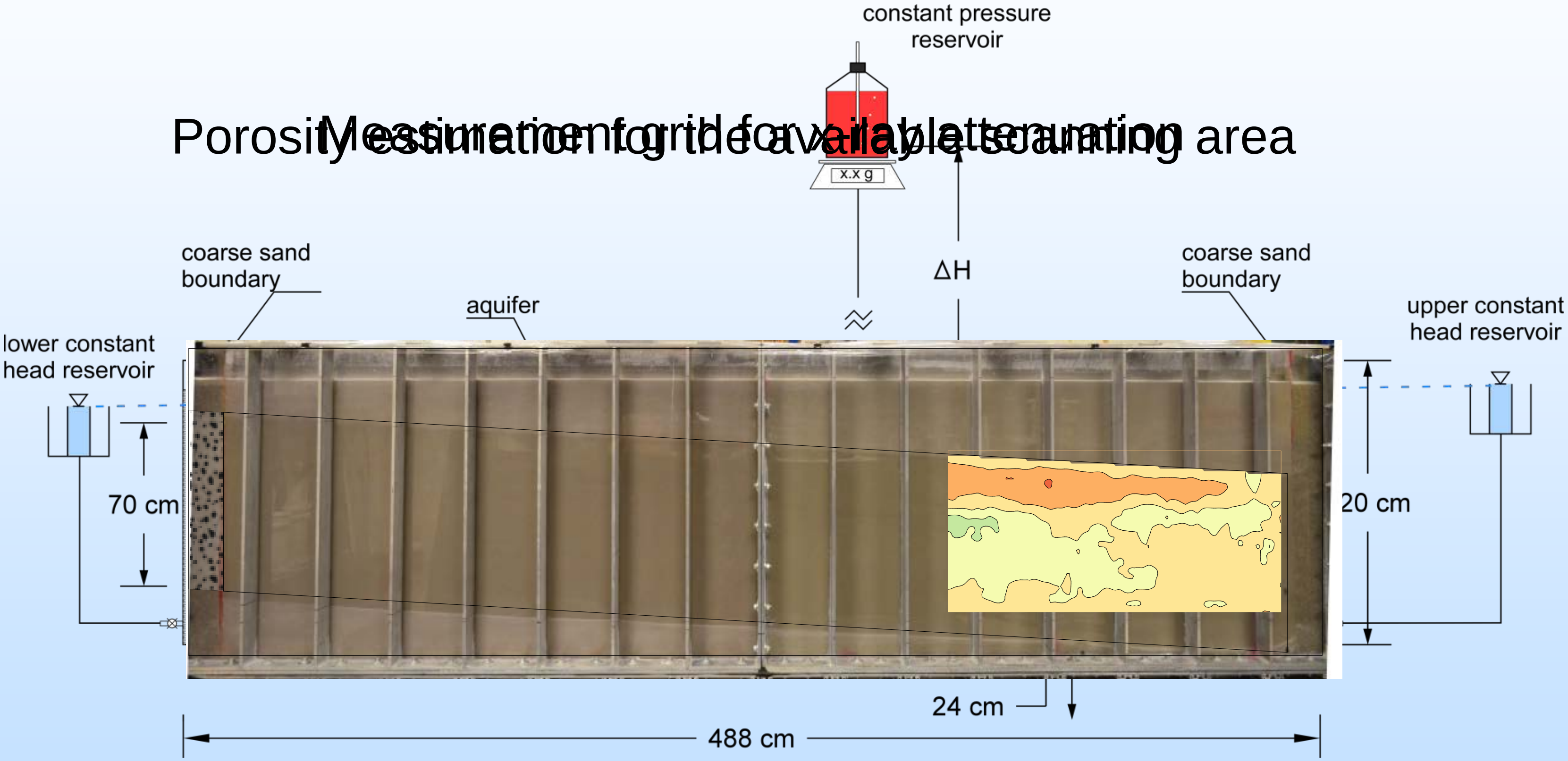
Ports for aqueous sampling



Large tank experiment

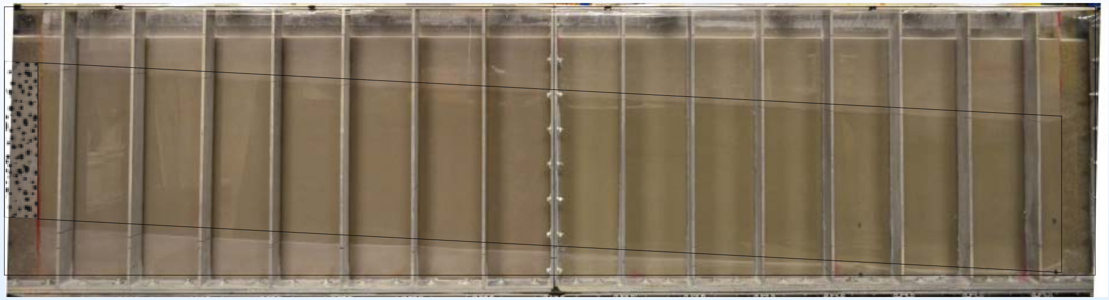
Porosity estimation for the available scanning area

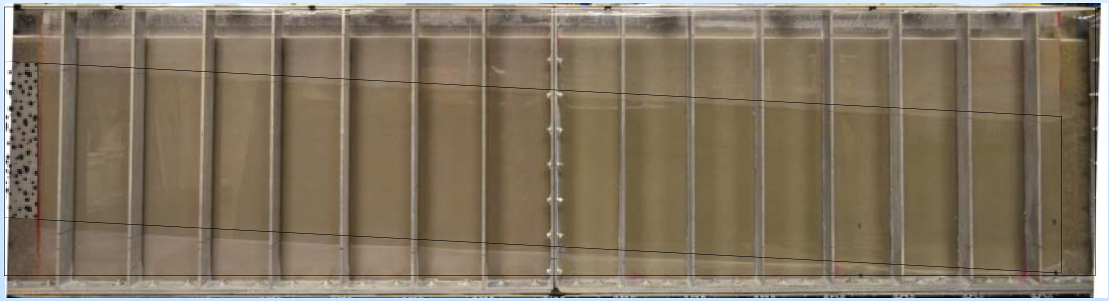
Measurement grid for x-ray attenuation



Modeling analog fluids with TOUGH2-T2VOC

Injection stage lasts 6 hours @ 6 ml/min
Redistribution simulated for 10 days





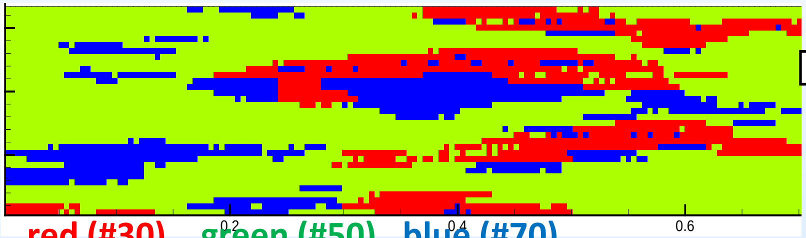
20.2 hrs of simulation for 10.4 hrs of injection

- ✓ Injection volume = 890 ml
- ✓ Injection flow rate = 1.43 ml/min (average)

Entrapment saturation distribution (3 days after injection)

Tank Experiments in Highly Heterogeneous Systems

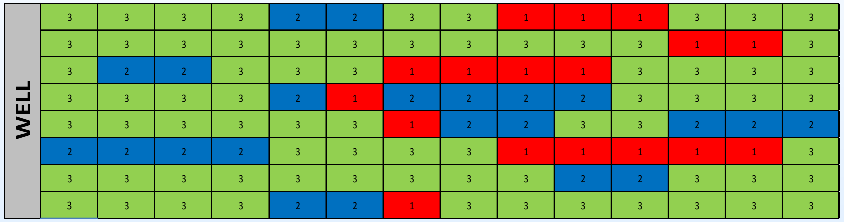
A computer-generated realistic heterogeneous aquifer



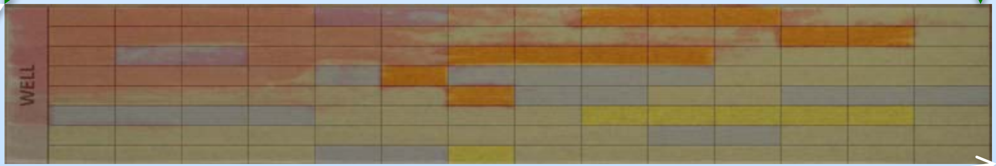
red (#30) **green (#50)** **blue (#70)**

Coarse **Medium** **Fine**

Simplified for packing



WELL	3	3	3	3	2	2	3	3	1	1	1	3	3	3
	3	3	3	3	3	3	3	3	3	3	3	1	1	3
	3	2	2	3	3	3	1	1	1	1	3	3	3	3
	3	3	3	3	2	1	2	2	2	2	3	3	3	3
	3	3	3	3	3	3	1	2	2	3	3	2	2	2
	2	2	2	2	3	3	3	3	1	1	1	1	1	3
	3	3	3	3	3	3	3	3	3	2	2	3	3	3
	3	3	3	3	2	2	1	3	3	3	3	3	3	3



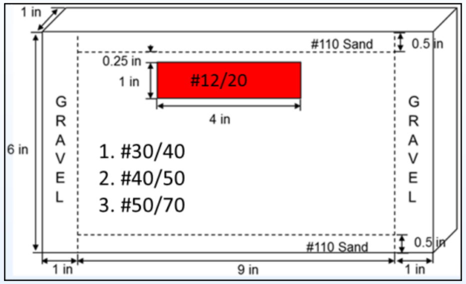
Tank data

Tank setup

Dissolution trapping

❑ Selection of analog fluids
❑ Small cell experiments
❑ Convective mixing
❑ Dissolution model development
❑ Large tank experiments (dissolution and low permeability zone storage)

2-D Small Tank Experiments: Homogeneous Media (water/propylene glycol)



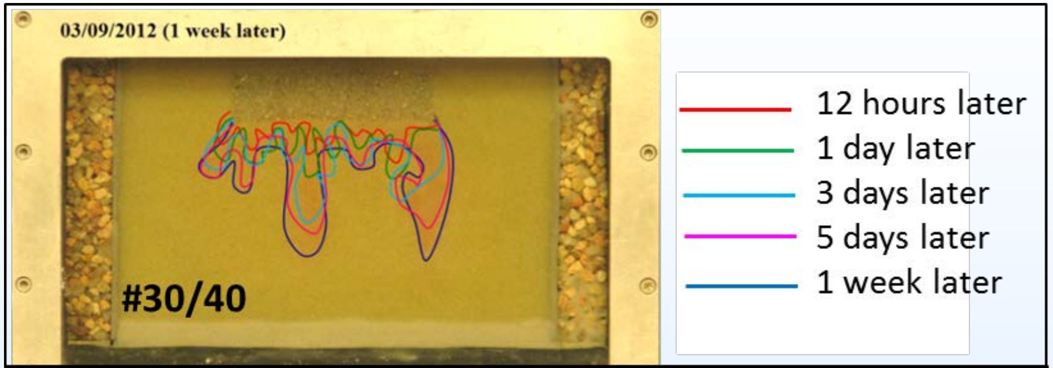
Rayleigh Number, Ra

$$Ra = \frac{k\Delta\rho g H}{D\mu\emptyset}$$

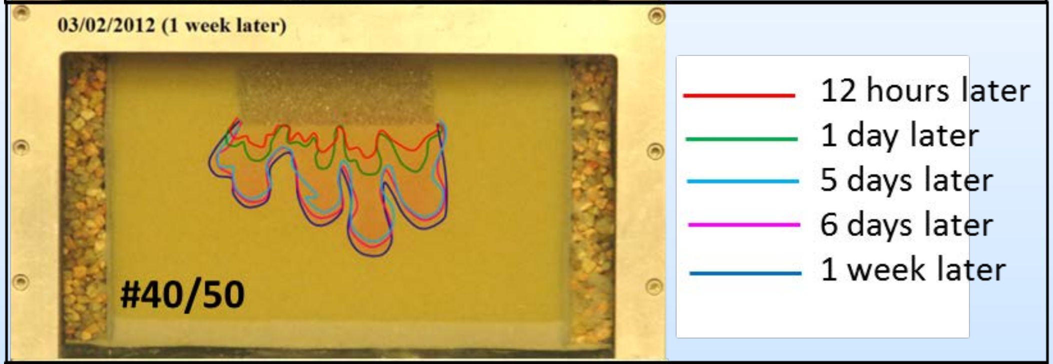
$$Ra_c > 4\pi^2(\sim 40)$$

Rayleigh Number for scrCO2-brine @ Typical Reservoir Conditions ~ 6 - 10^3

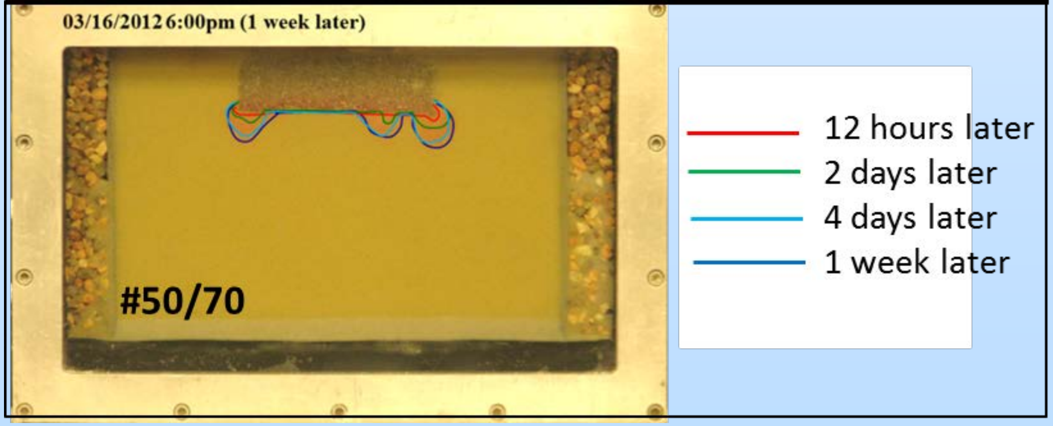
Ra


03/09/2012 (1 week later)

451

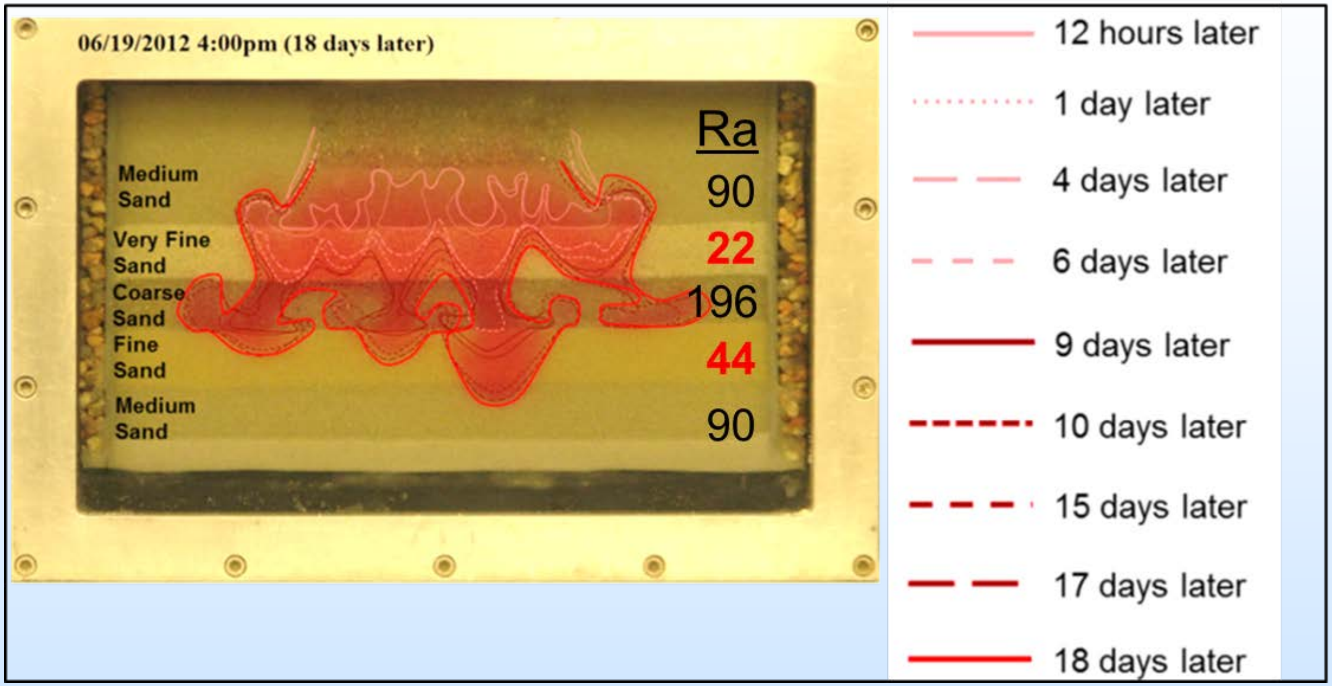

03/02/2012 (1 week later)

221

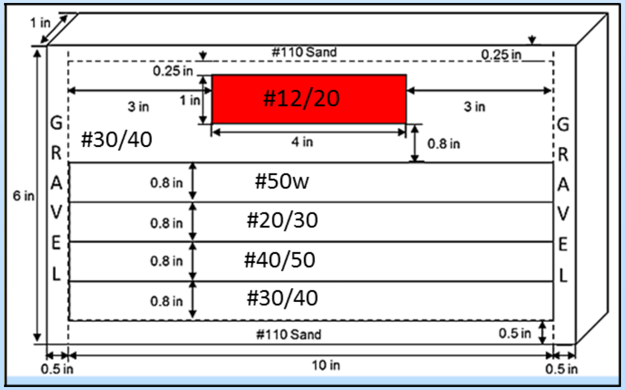

03/16/2012 6:00pm (1 week later)

138

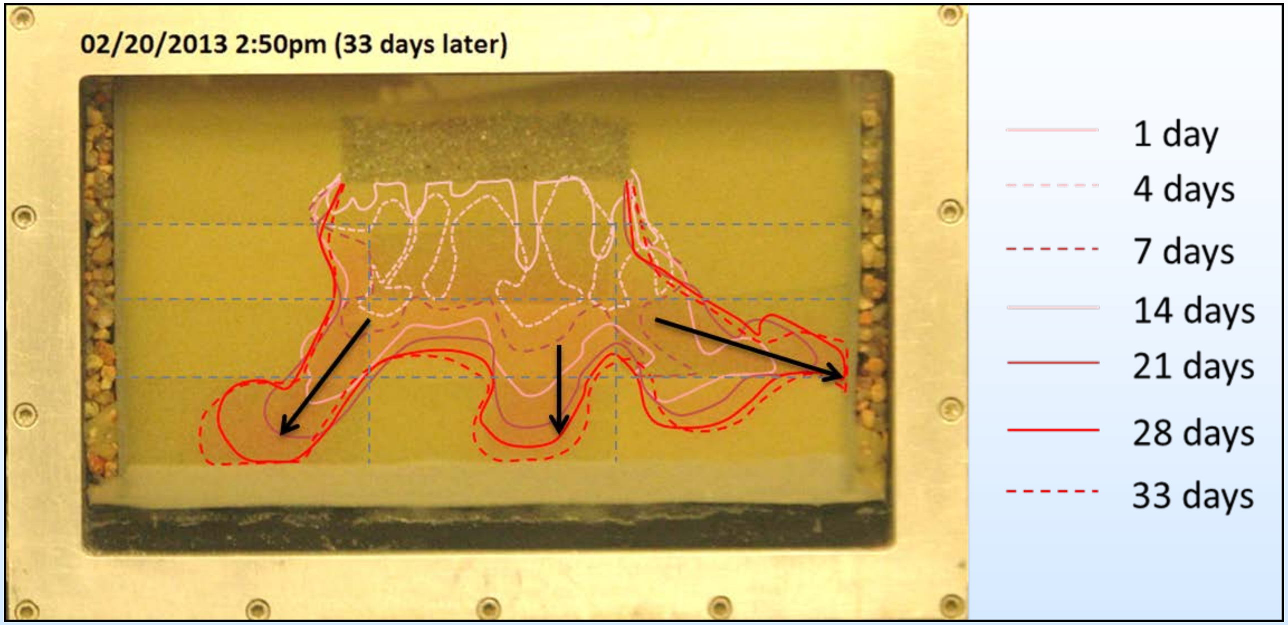
2-D Small Tank Experiments: Heterogeneity effect on density-driven fingering (water/propylene glycol)



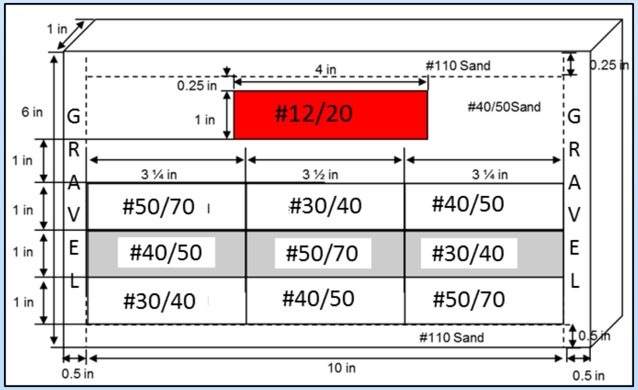
In the transition of high-permeable medium and low permeable medium, characteristics of fingered flow tends to change due to merging of fingers



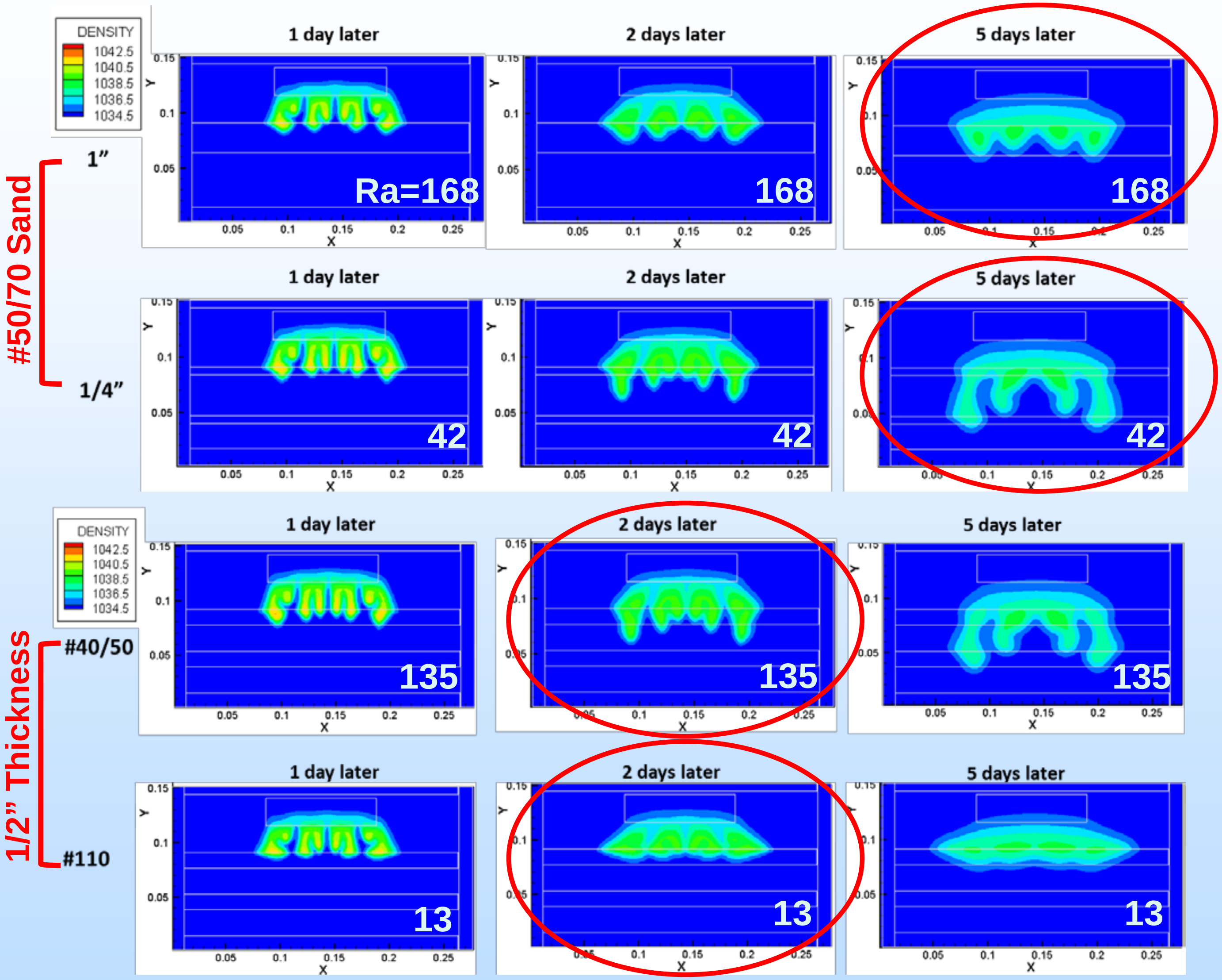
2-D Small Tank Experiments: Heterogeneity effect on density-driven fingering (water/propylene glycol)



Convective mixing controlled by density driven sinking through high permeability connected pathways



Numerical Modeling: Layered Heterogeneous Formations having Low Permeability Zones



Rayleigh Number for scrCO2-brine @ Typical Reservoir Conditions ~ 6 - 10^3

Accomplishments

- ☐ 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
  - ✓ Simulated the two-phase flow in small tank experiments and compared the model results with experimental data
  - ✓ Developed a new multiphase flow solver (based on the Finite Volume method) for analysis of the experimental data and new constitutive models and non-equilibrium mass transfer
  - ✓ 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 models based on the classical two-phase flow theory were able to capture the main features observed during the migration of the ScCO2 surrogate fluid in the small tanks**
- **Selection of appropriate relative permeability curves was critical to predict dynamic changes in the surrogate fluid distributions**
- **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 in intermediate-scale.**
- **Convective mixing due to density-driven finger flow in highly heterogeneous formations appears to be not important.**
- **Our experimental results and literature show that the residual non-wetting phase saturation is strongly function of the saturation at the end of injection.**

Future Efforts

☐ **Obtain more 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.**

☐ **Intermediate-scale heterogeneous experiments and models involving both capillary and dissolution trapping.**

☐ **Update model parameters with measured relative permeability curves in separate homogeneous column tests.**

☐ **Continue developing/testing the constitutive models with hysteresis against experimental data.**

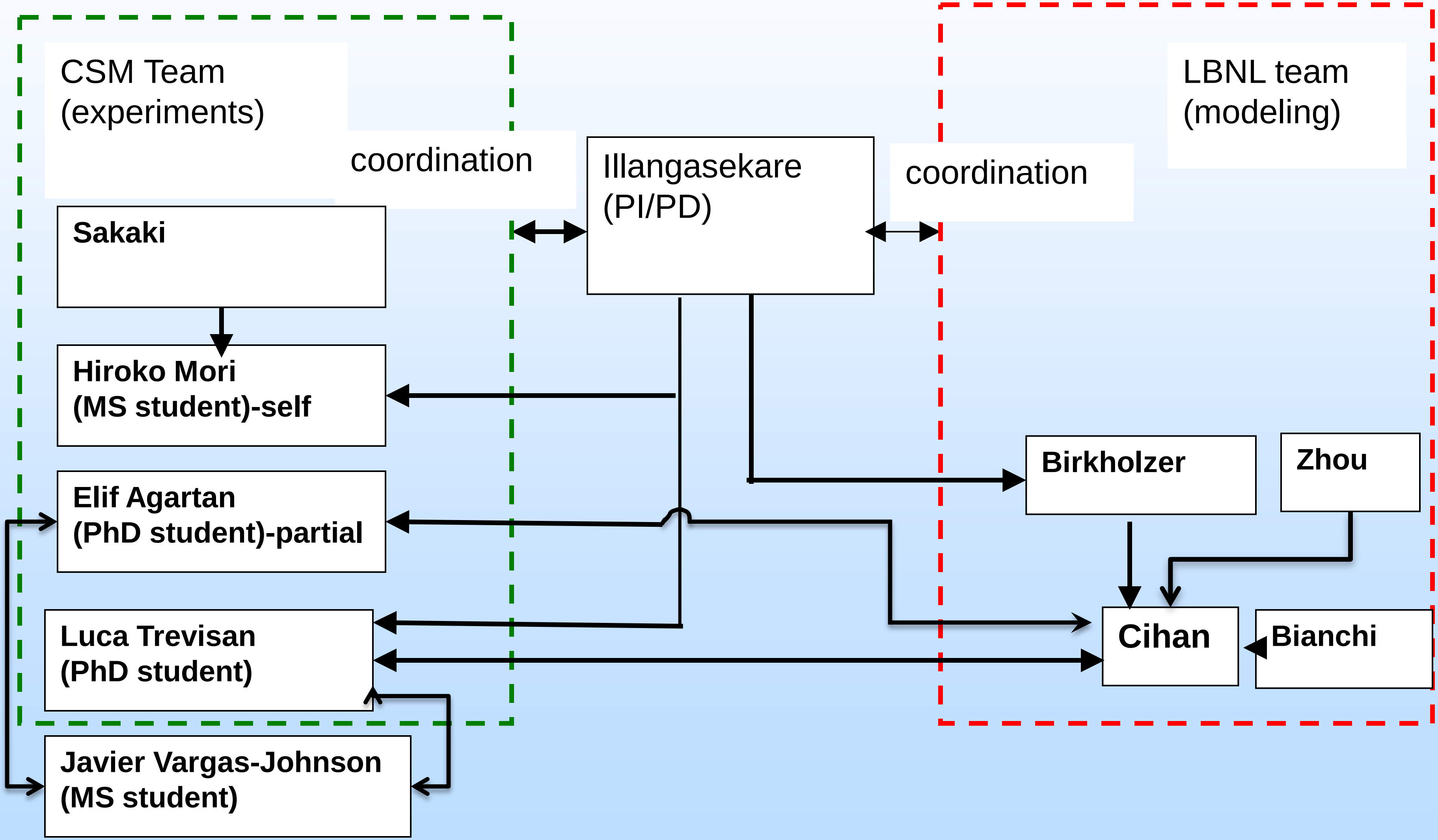
☐ **Improve the numerical models by incorporating the validated constitutive models**

Appendix

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

Organization Chart

1. Scientific & Technical Merit
2. Existence of Clear, Measurable Milestones
3. Utilization of Government Resources
4. **Technical Approach**
5. Rate of Progress
6. Potential Technology Risks Considered
7. Performance and Economic Factors
8. Anticipated Benefits, if Successful
9. Technology Development Pathways



CSM Team
(experiments)

coordination

Illangasekare
(PI/PD)

coordination

LBNL team
(modeling)

Sakaki

Hiroko Mori
(MS student)-self

Elif Agartan
(PhD student)-partial

Luca Trevisan
(PhD student)

Javier Vargas-Johnson
(MS student)

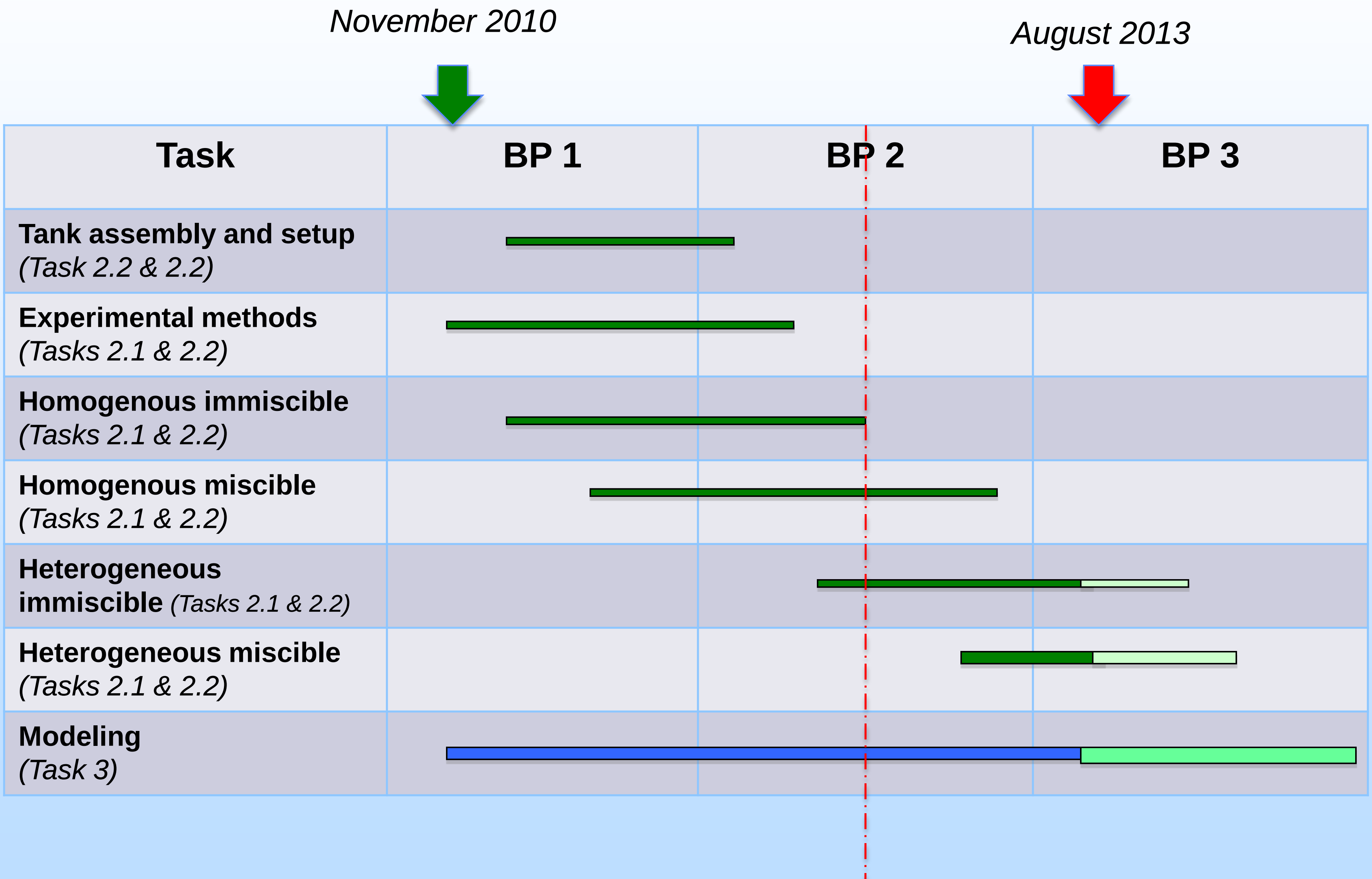
Birkholzer

Zhou

Cihan

Bianchi

Project Overview:
Schedule



November 2010

August 2013

Task	BP 1	BP 2	BP 3
Tank assembly and setup *(Task 2.2 & 2.2)*			
Experimental methods *(Tasks 2.1 & 2.2)*			
Homogenous immiscible *(Tasks 2.1 & 2.2)*			
Homogenous miscible *(Tasks 2.1 & 2.2)*			
Heterogeneous immiscible *(Tasks 2.1 & 2.2)*			
Heterogeneous miscible *(Tasks 2.1 & 2.2)*			
Modeling *(Task 3)*			

Bibliography

- Cihan, A., Birkholzer, J., Bianchi, M., Zhou, Q., Illangasekare, T. H., Trevisan, L., “A New Connectivity-Based Upscaling Methodology for Multi-Scale Two-Phase Flow Processes in Heterogeneous Geological Formations”, the CCUS 12th Annual Conference, Pittsburgh, PA, May 13-16 2013.

- Cihan, A., Birkholzer, J., Illangasekare, T. H., Zhou, Q., “A Theoretical Approach to Represent Hysteresis in Capillary Pressure-Saturation Relationship Based on Fluid Connectivity in Void Space”, submitted to Water Resources Research.

- Agartan, E., T.H.Illangasekare, A. Cihan, J. Birkholzer, Q. Zhou, L. Trevisan, 2013.A Fundamental Study of Convective Mixing of CO2 in Layered Heterogeneous Saline Aquifers using Surrogate Fluids in Laboratory Tanks and Numerical Modeling, to be submitted to J. of Green House Gases.

- Mori,H., L. Trevisan, T. Sakaki, A. Cihan, K. M. Smits, and T. H. Illangasekare, 2013.Measurement and evaluation of the relationship between capillary pressure, saturation, and relative permeability for carbon sequestration model, in preparation.

- Trevisan, L., Cihan, A., Birkholzer, J., Q.Zhou. And Illangasekare, T. H., 2013. Investigation of mechanisms of supercritical CO2 migration and trapping in deep saline reservoirs using surrogate fluids at ambient laboratory settings