Systems Modeling & Science for Geologic Sequestration

Project Number: LANL FE10-003 Task 3

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Carbon Storage R&D Project Review Meeting
Developing the Technologies and
Infrastructure for CCS

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Collaborators

- Tissa Illangasekare (Colorado School of Mines)
- Michael Plampin (Colorado School of Mines)
- Jeri Sullivan (LANL)
- Shaoping Chu (LANL)
- Jacob Bauman (ATK)
- Mark Porter (LANL)
- Elizabeth Keating (LANL)
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Presentation Outline

- Benefit to the program
- Project overview
- Project technical status
- Accomplishments to date
- Future Plans
- Appendix

Benefit to the program

- Program goals being addressed:
  - Develop and validate technologies to ensure 99 percent storage permanence.
  - Develop technologies to improve reservoir storage efficiency while ensuring containment effectiveness.
- Project benefit:
  - This project is developing system modeling capabilities that can be used to address challenges associated with infrastructure development, integration, permanence & carbon storage options. The project is also developing science basis that can be used to assess impacts of CO_2 leakage in shallow aquifers. This technology contributes to the Carbon Storage Program's effort of ensuring 99 percent CO_2 storage permanence in the injection zone(s).

Project Overview:
Goals and Objectives

1. Develop and apply system modeling capabilities applicable to CCS storage operations:
   - Develop capabilities that can be used to evaluate water production and treatment for beneficial reuse.
   - Develop system modeling capabilities for assessment of feasibility of long-term CO_2 storage at CO_2-EOR sites
2. Characterize multi-phase CO_2 flow in groundwater aquifers through an integrated experimental-simulation approach
3. Characterize multi-phase CO_2-brine flow through faults

Technical Status

Water Treatment Module

Water production and treatment for beneficial reuse

- If or when water is extracted to minimize risks during geologic CO_2 storage, what do we do with it?
  - Can it be treated for multiple uses, while minimizing energy use, costs, and maximizing storage efficiencies?
  - Can we incorporate this into a systems model so that we can predict costs, risks, and effectiveness for a variety of potential site conditions?
- Approach
  - Develop system modules for doing assessment while taking into account complexities (integrate with CO_2-PENS)
  - Apply model using real-world data from literature and from accepted water treatment practices worldwide
- Complexities
  - Water types and sources are different and chemically more complex than typical waters treated for municipal and industrial use.
  - Obtaining complete cost data is difficult.
  - Costs and ancillary benefits are very specific to the capture/storage technology realm.

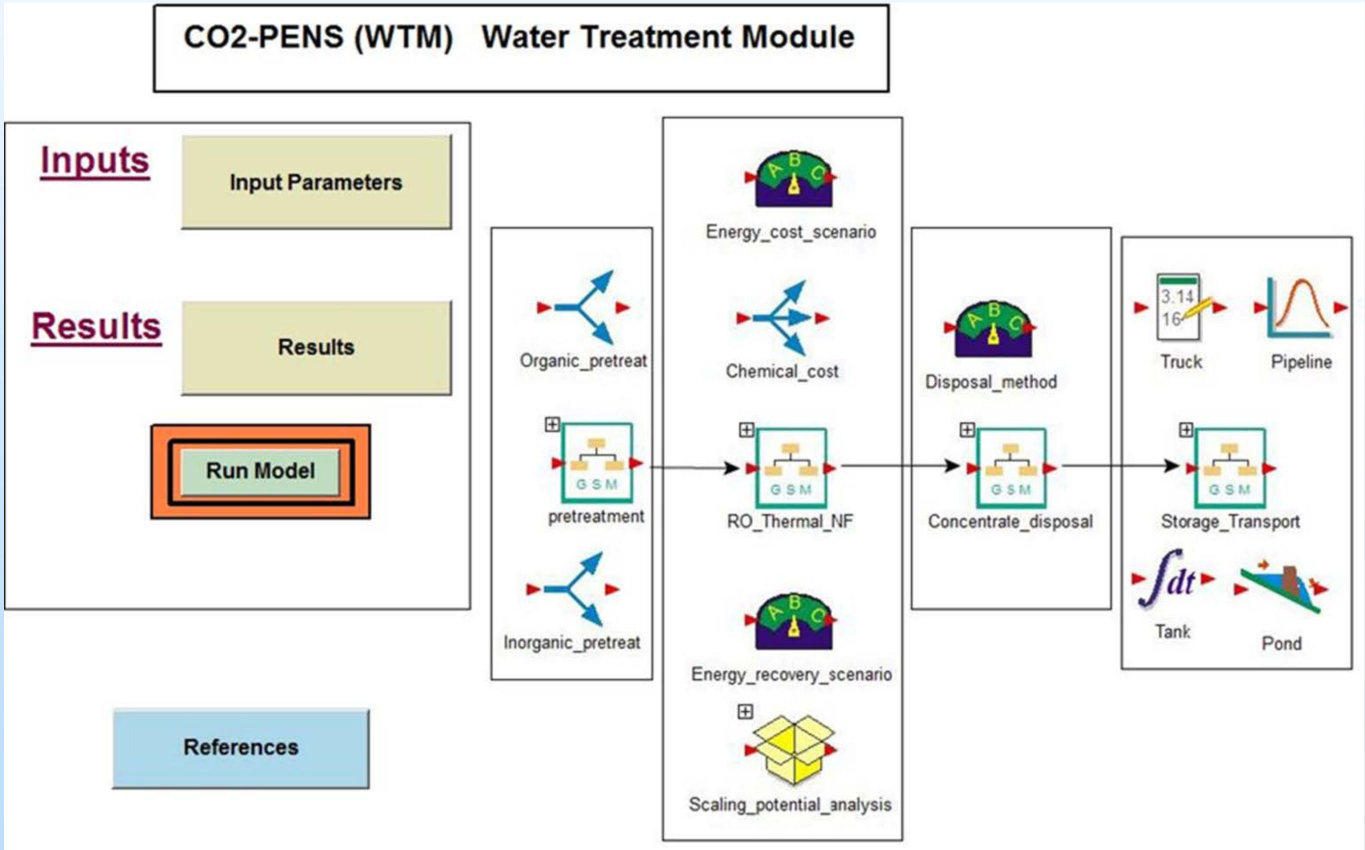
WTM effort focus

- Progress till FY14:
  - Developed WTM and demonstrated its applicability using various field data
- FY14 Tasks:
  - Verify the cost profile of the WTM versus an engineering-type model (Desalination Energy Evaluation Program-DEEP) using site-specific data
  - Understand impact of various factors to overall costs
  - Develop a reduced order model (ROM) to predict brine displacement due to CO_2 injection
  - Link WTM to CO_2-PENS

WTM

The module includes four main parts:

1. Pretreatment (organic, inorganic)
2. Main treatment processes (RO, thermal (MSF or MED-TVC), and NF methods)
3. Concentrate disposal (with various methods depends on location; water type, quality and volume)
4. Storage (tank, pond) and transport (pipeline, truck, etc)



Completed incorporation of transportation costs and energy recovery benefits in FY14

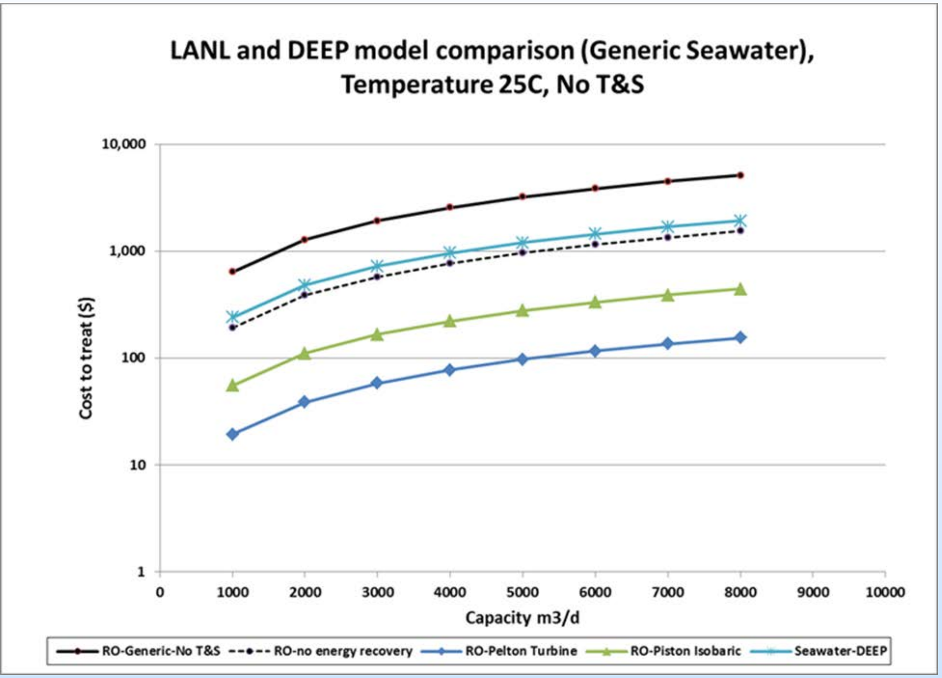
Comparison with DEEP

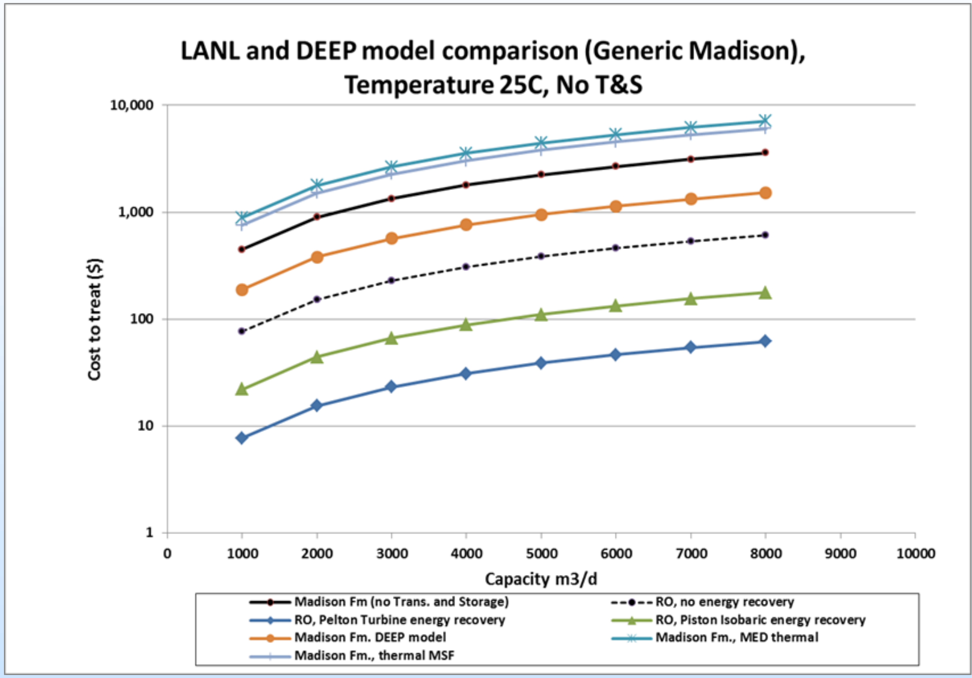
- DEEP: Engineering based calculations, such as capital and O&M costs, infrastructure depreciation over a project lifetime, and economies of scale for treatment
- Goal is to compare overall treatment costs
- Goal is not to reproduce engineering complexities of DEEP but assure cost estimates reflect realistic factors

Water quality scenarios, input and output data, and model criteria used for model simulations.

Location	Seawater	Rock Springs Uplift, Madison Fm., Wyoming
Plant Type	Saline Water RO	Brackish Water RO Saline Water MED and MSF
Formation Type	Average Surface Seawater	Brackish to Saline Fm; Gas Reservoir
Feed Volume[1] (m^3/d)	37,854 (10 mgd)	37,854 (2000-10,000[#]) (10 mgd)
Supply TDS (mg/L)	35,000	<1,000-76,777 Mean Brackish=14,114 High=Brine 1
Pretreatment Type	Model Selected	Model Selected
Permeate % of feed volume	50	50[#]
Desired Permeate TDS (mg/L)	<500	<500-1500
Concentrate as % of feed volume	50	50[#]
Concentrate TDS (mg/L)	Model Output	Model Output
Cost to Treat (US$/$m^3$)	Model Output	Model Output
Temperature range (°C)	25	49-117; 25 (base case)
Estimated cost of energy (US$/kWh)	0.07	0.04-0.20
Feed pH	7	6.0-8.6
Feed Turbidity (NTU)	5	0.5-10
Feed Silt Density Index	5	0.5-10

Comparison with DEEP

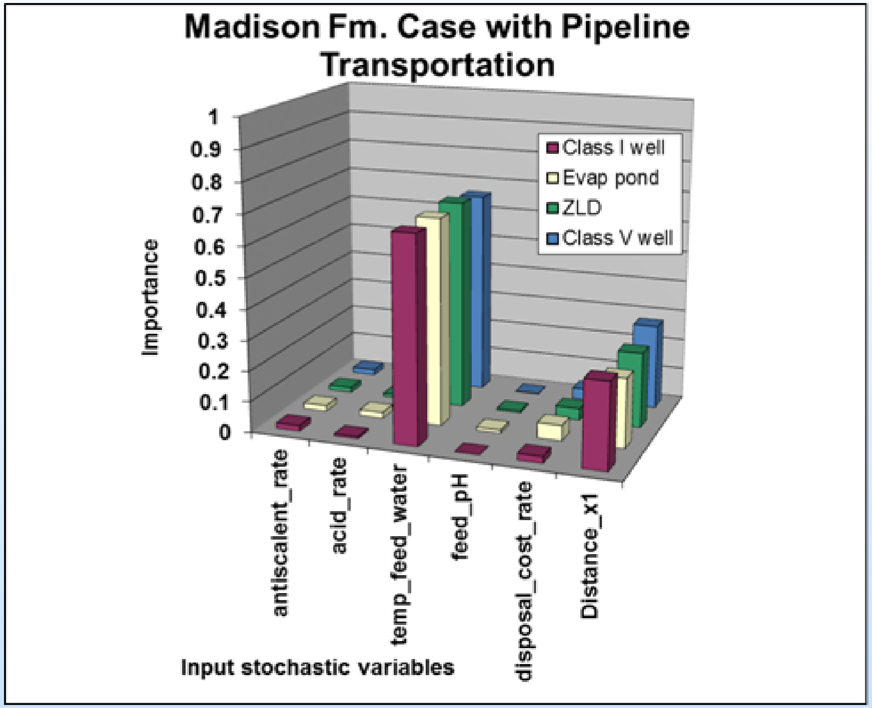




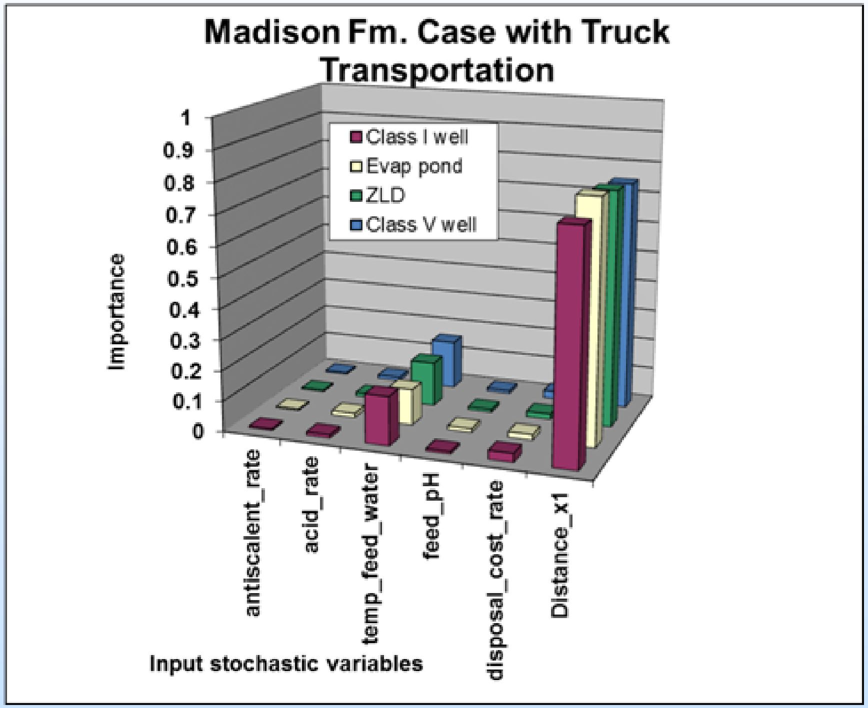
Base model includes 50% recovery, no organic pre-treatment, no transportation, no storage

WTM provides results to assess impact of uncertain factors on total costs

Conditions include TDS= 14,000 mg/L; T= 15-45°C for RO, 45-65°C for thermal methods.



Madison Fm. Case with Pipeline Transportation



Madison Fm. Case with Truck Transportation

- Feed temperature most important factor followed by transportation distance
- Feed temperature controls the selection of treatment method in WTM
- Thermal methods are selected at T >45°C because of potential damage to RO or NF membranes

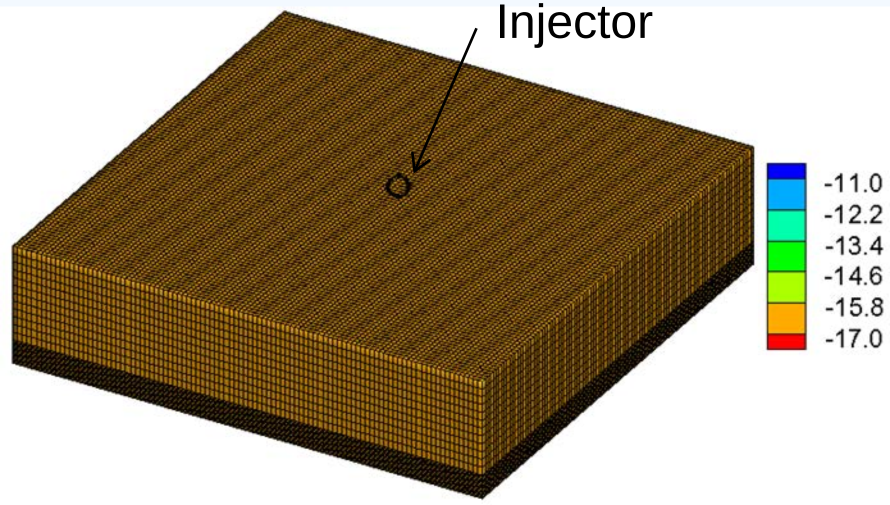
- Greater importance on distance than on feed temperature.
- If truck transportation is used, reducing distances is critical to cost management

Reduced Order Model for brine production

- Goal: Develop a reduced order model to calculate amount of brine produced due to CO_2 injection
  - Provide input to WTM
  - Account for variability in reservoir parameters, injection rates
  - Couple to CO_2-PENS along with WTM

Approach

- Monte-Carlo simulations of CO_2 injection using FEHM



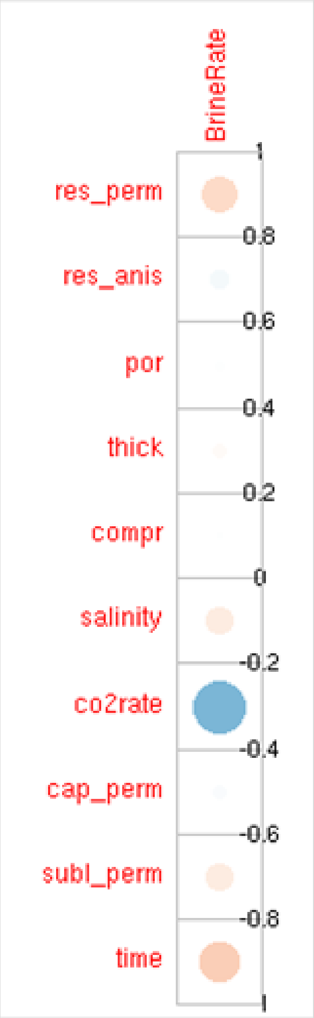
- 10km x 10kmx250m
- Grid block dimension (100m x 100m)
- 50 m thick reservoir, 40 m caprock and a 80 m sublayer
- 3,10, 30 years CO_2 injection followed by 27, 100, 270 years of post-injection period
- Constant-pressure boundaries

- ~300 realizations sampling multiple uncertain parameters
- Sensitivity analysis of simulation results
- Response surface correlating brine production rate to uncertain parameters

Uncertain parameters

Uncertain parameters		Min	Max	Distribution
Reservoir	Thickness (m)	50.0	200.0	50, 100, 200
	Permeability (mD)	10.0	215.2	Uniform
	Permeability anisotropy (Kv/Kh)	0.01	0.22	Uniform
	Porosity	0.05	0.20	Uniform
	Pore compressibility	5E-4	2E-2	Uniform
	CO_2 injection rate (kg/s)	10.0	5000.0	Uniform
	Salinity	10.0	230.0	Uniform
Confining rocks	Permeability (mD)	1e-5	1e-2	Uniform
	Sublayer Permeability	1e-5	1e-2	Uniform
	Caprock thickness 40m			

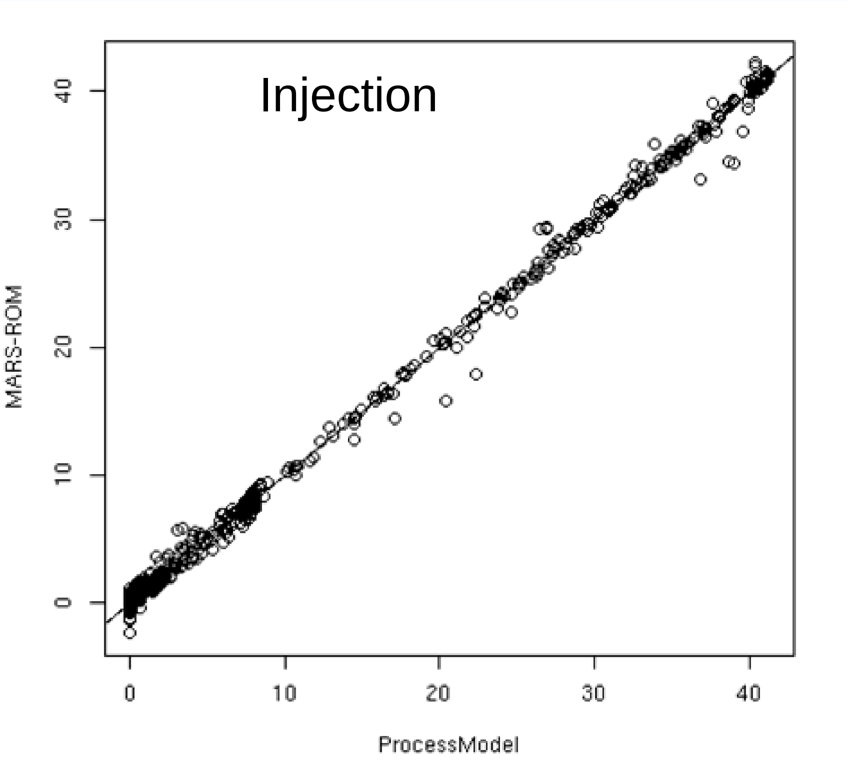
Sensitivity Analysis

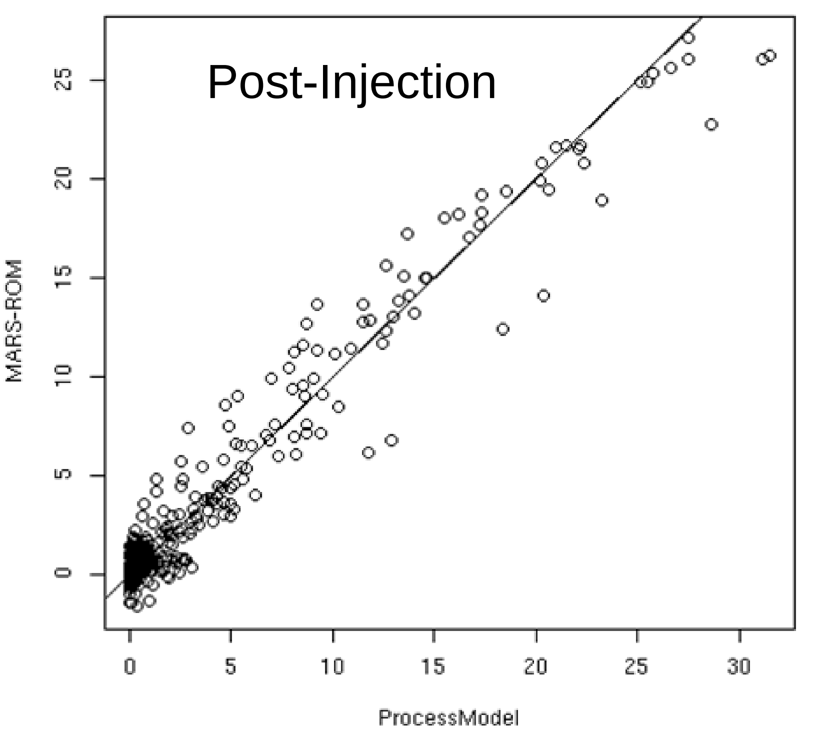


Brine production rate most sensitive to injection rate, reservoir and caprock permeability, salinity

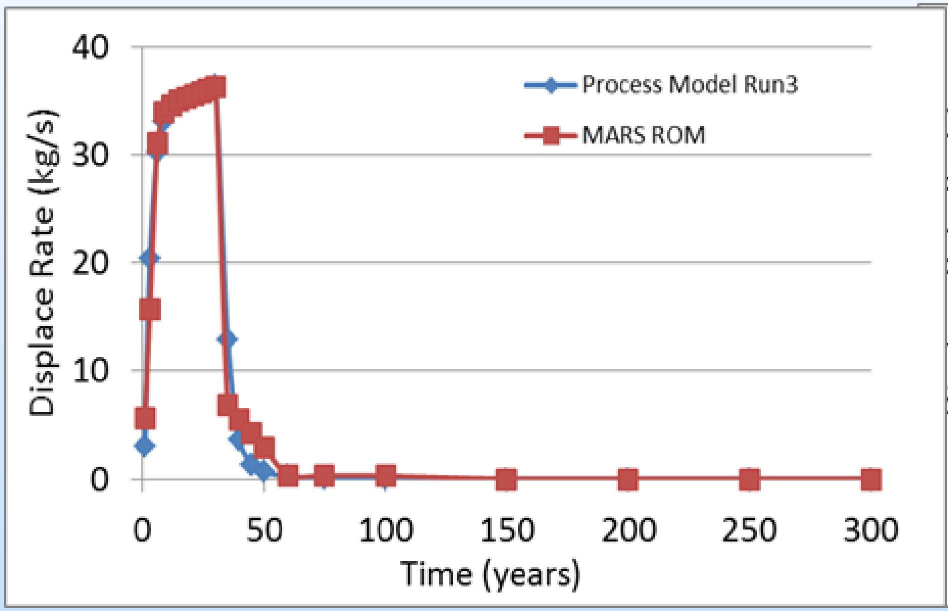
Reduced Order Model

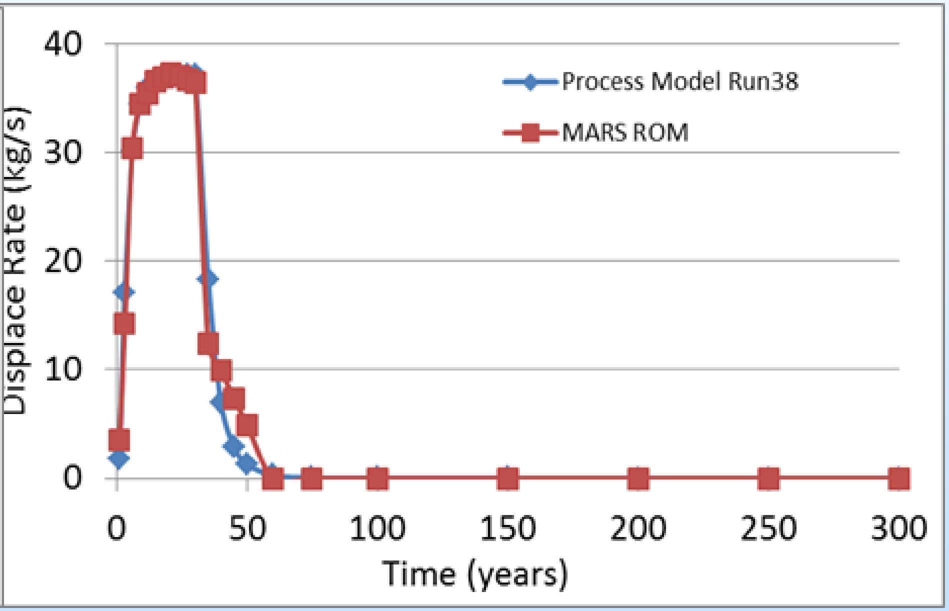
- Two stage approach: injection data and post-injection data





ROM prediction





Next Steps

- WTM and brine production ROM are being linked to CO_2-PENS
- Stand-alone WTM model will be publicly available (contact spchu@lanl.gov on availability)

Characterization of CO_2-water multi-phase flow

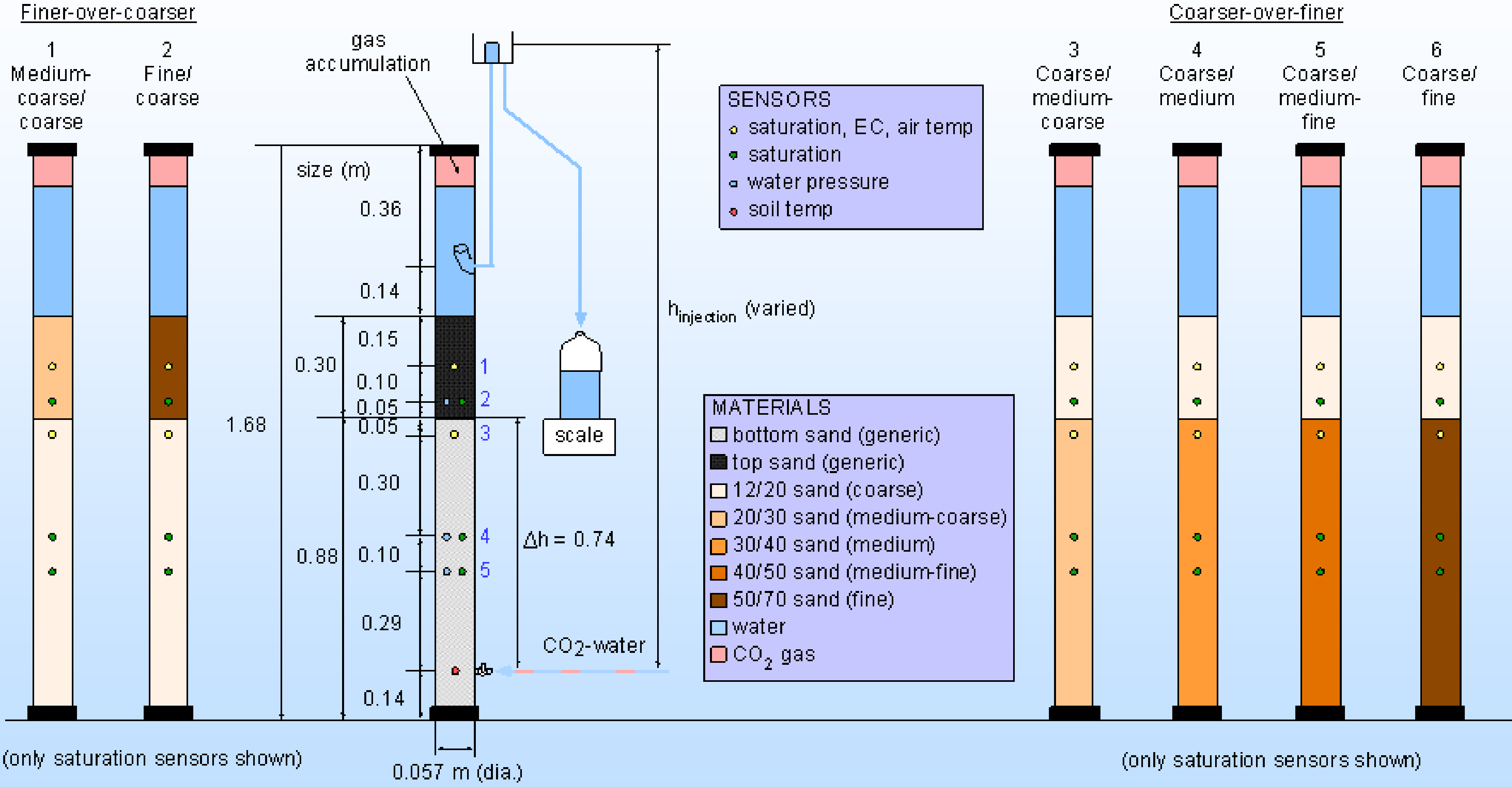
Characterization of CO_2-water multi-phase flow

- To characterize the impacts in shallow aquifer subsequent to potential leakage of CO_2 and CO_2-dissolved water it is necessary to understand the process of gas exsolution, gas phase expansion and subsequent migration
  - Factors affecting the spatiotemporal evolution of CO_2 gas phase
  - Effect of heterogeneity in large systems
  - Generate data to develop theory behind multi-phase flow process when gravity & capillary forces are critical
- Integrated approach
  - Demonstrate real-world applications and upscaling effects through intermediate scale experiments
  - Experiments under controlled conditions where CO_2-dissolved water is injected through sand columns/tanks under different conditions
    - Collaboration with Prof. Tissa Illangasekare at Colorado School of Mines (CSM): unique, world-class experimental facility at CSM
  - Experimental results used to develop models in LANL's FEHM simulator

Characterization of CO_2-water multi-phase flow

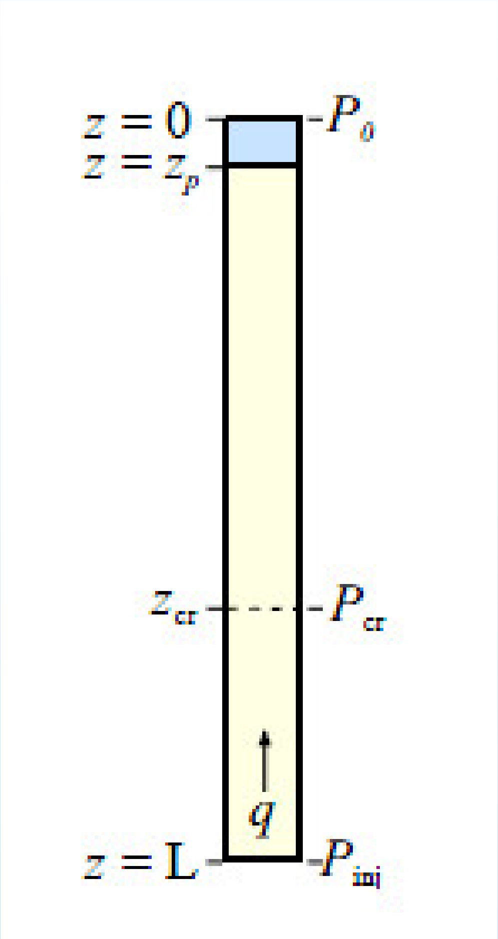
- Status pre-FY14:
  - Completed multiple long (4m) and short (1.36m)1D column & pseudo-2D column experiments
  - Results showed that:
    - Heterogeneity has a strong effect on the spatiotemporal evolution of gas phase.
    - Interfaces from one type of sand to another can enhance the growth of gas phase, when the heterogeneity exists at a location where the injected water is oversaturated with CO_2.
- FY14:
  - Numerical simulation of column experiments
  - Preparation of 2-D tank experiments

Column experiments to characterize effect of heterogeneity



Performed 35 different experiments: multiple injection pressures for each packing configurations

Critical pressure for gas-phase evolution



Thermodynamic equilibrium suggests that gas phase should evolve when pressure is equal to saturation pressure

$$P'_{cr} = P_{sat} - \Delta P_{flow}$$

Pressure drop due to flow

$$P'_{cr} = P_{sat} + \frac{\mu q (L - z_p)}{k}$$

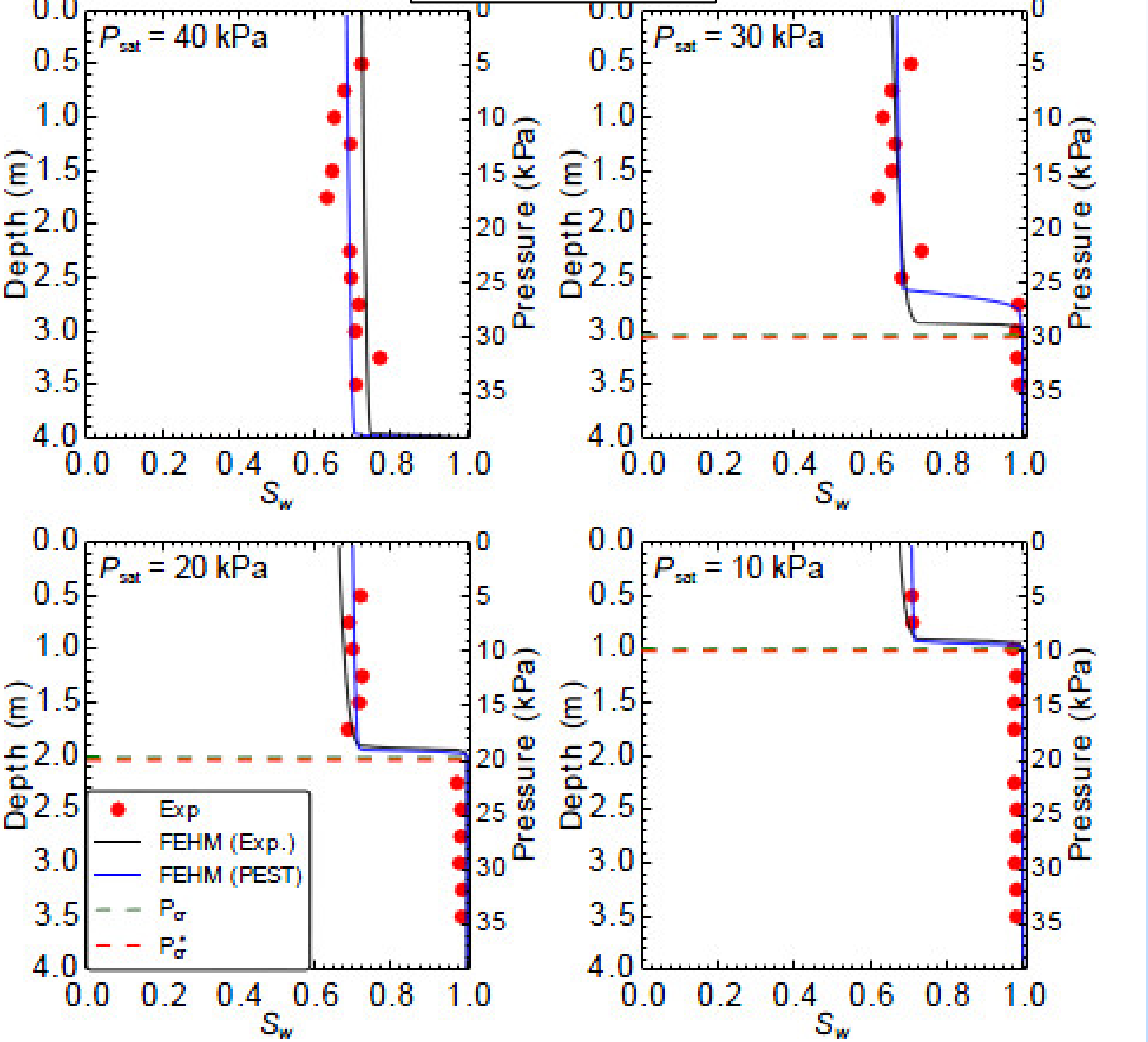
Homogeneous Sand

$$P'_{cr} = P_{sat} + \frac{\mu q (L - z_p)}{k_{eff}}$$

Heterogeneous Sand

Numerical simulations of column experiments using FEHM

Coarse sand

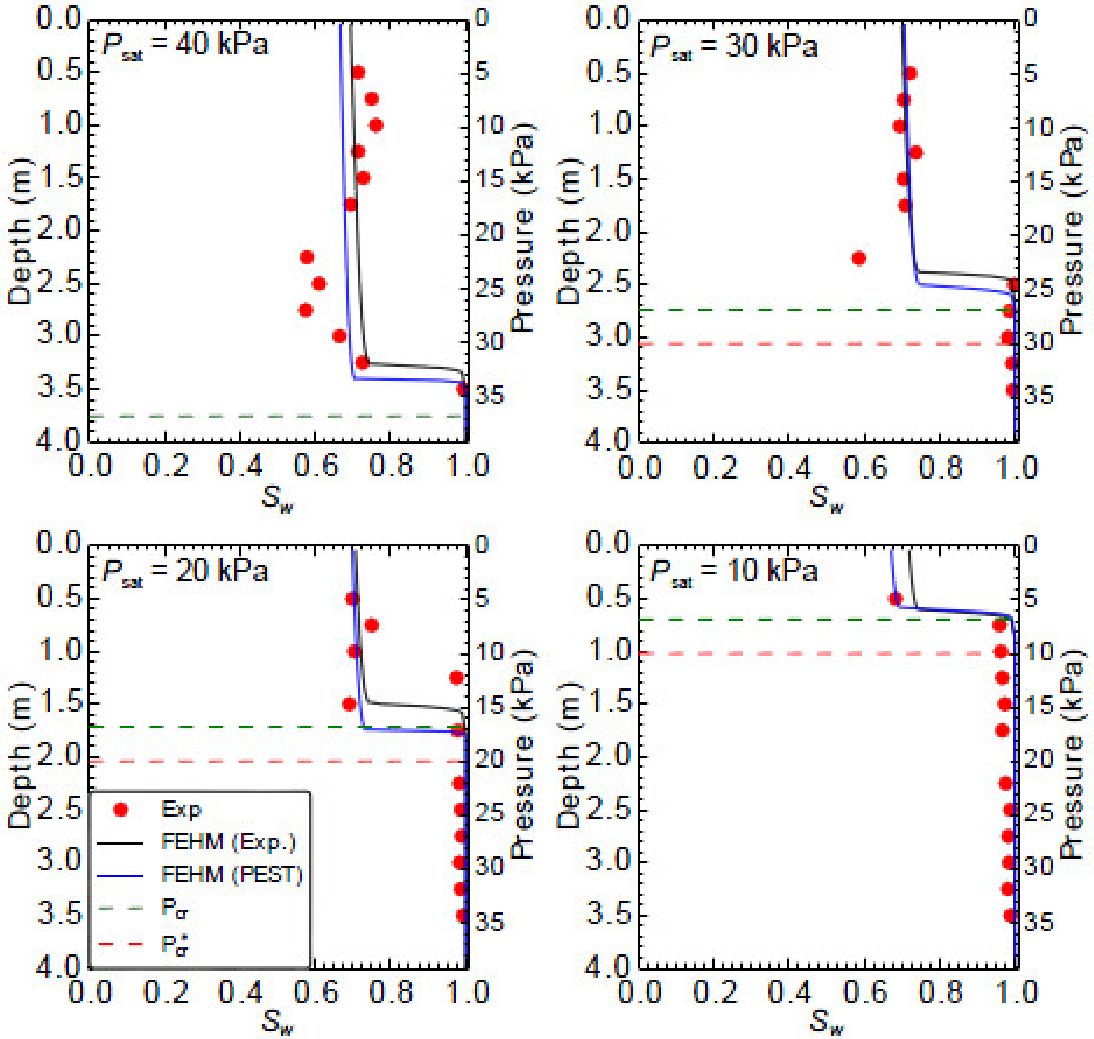


$$P^*_\sigma = P_{sat}$$

$$P_\sigma = P'_{cr}$$

Numerical simulations of column experiments using FEHM

Fine sand

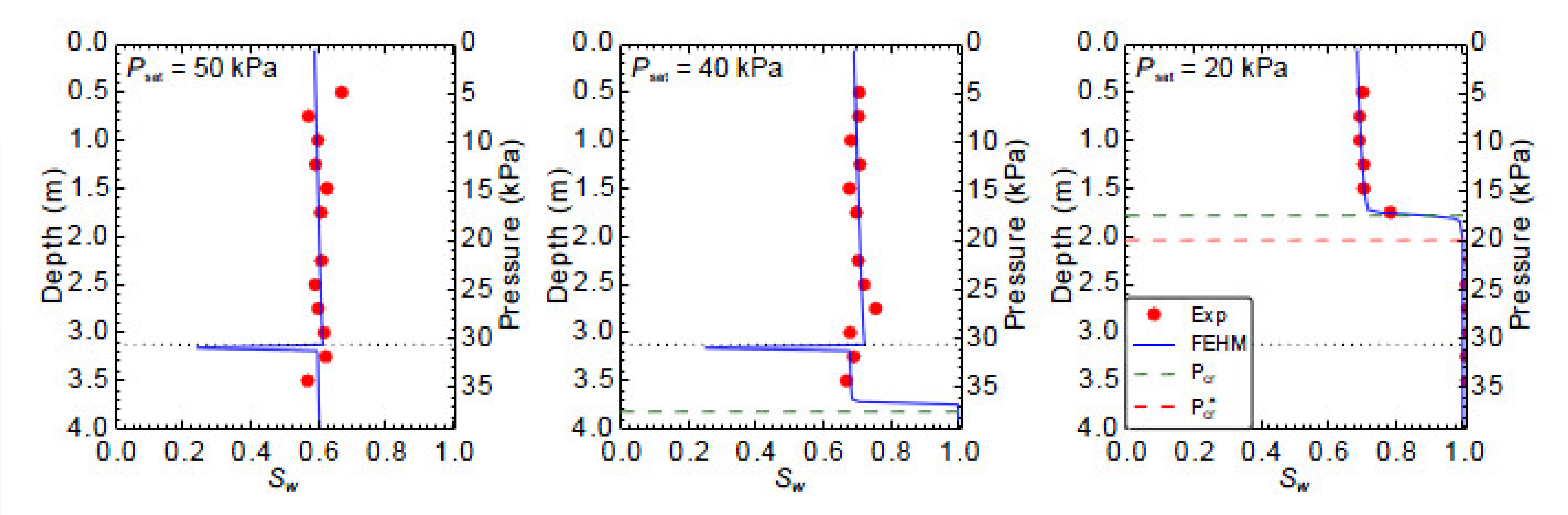


$$P^*_\sigma = P_{sat}$$

$$P_\sigma = P'_{cr}$$

Numerical simulations of column experiments using FEHM

Coarse-fine sand



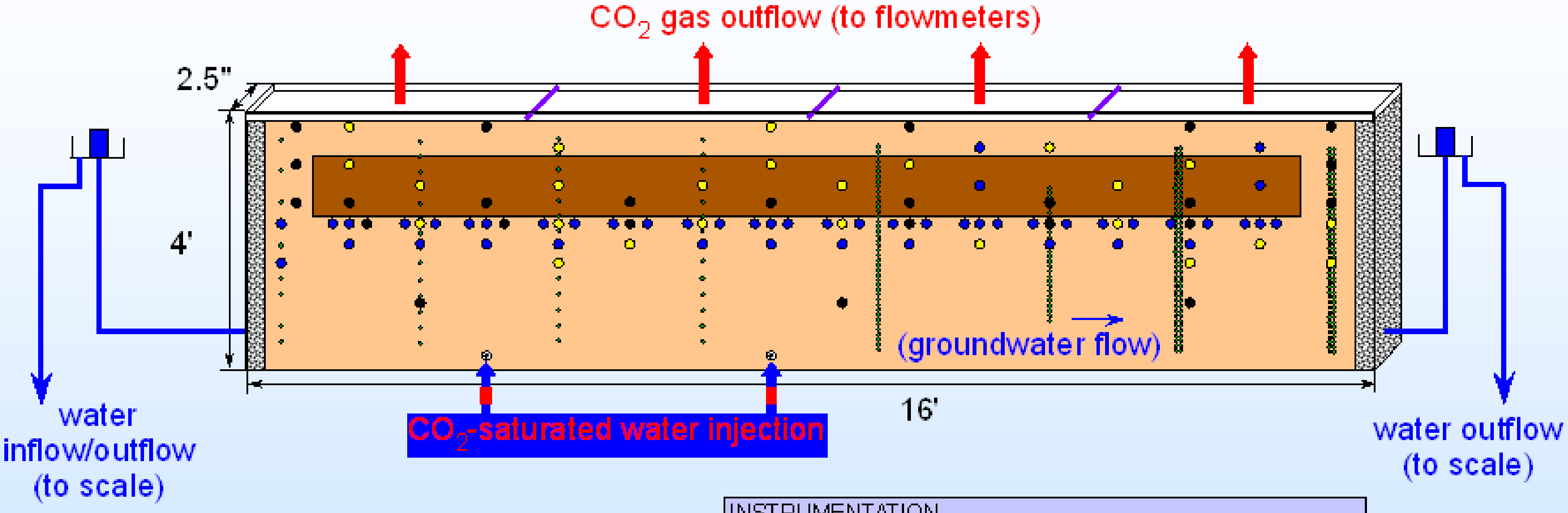
$$P_\sigma = P'_{cr}$$

$$P^*_\sigma = P_{sat}$$

Next Steps

- 2-D tank experiments and modeling

2-D tank experiments



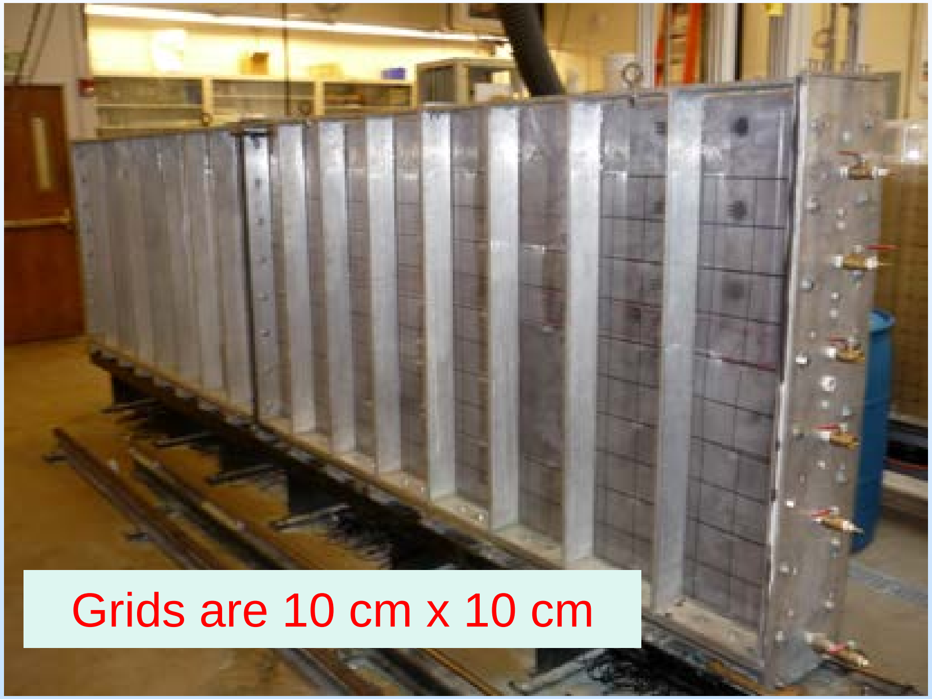
MATERIALS

- / plastic baffle
- 🟧 coarse sand (Granusil #20/30)
- 🟫 clay and/or fine sand
- ▨ gravel boundary (Granusil #8)
- ☐ headspace (air and/or CO_2 gas)
- ⊛ injection well

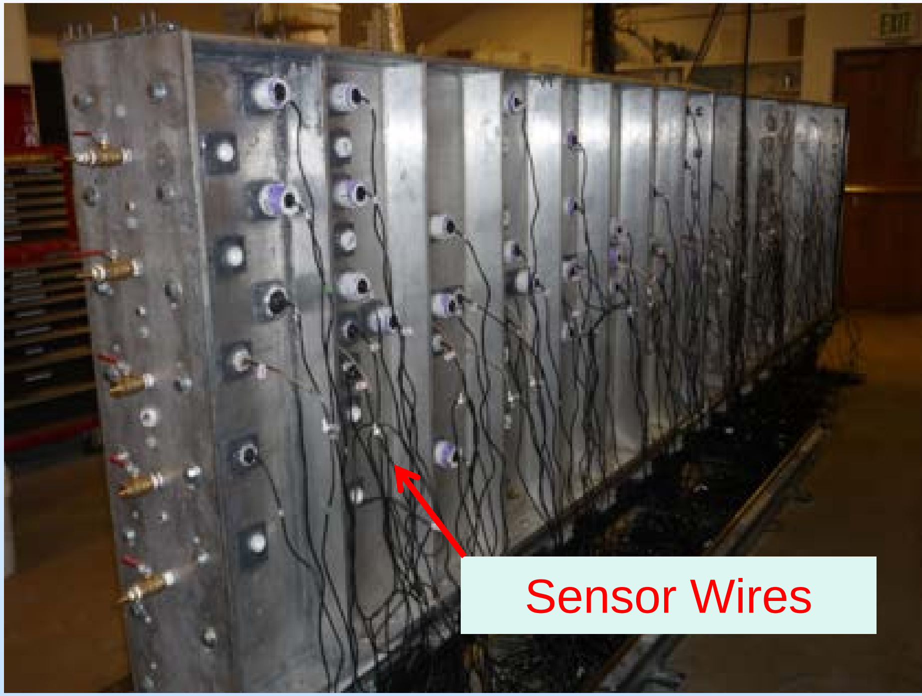
INSTRUMENTATION

- 🔵 saturation sensor (EC-5)
- 🟡 saturation & temperature sensor (EC-TM)
- ● saturation, EC, & temperature sensor (5TE)
- · sampling port (for measuring dissolved CO_2 concentration)

2-D tank experimental setup


Grids are 10 cm x 10 cm

Plexi-glass Wall


Sensor Wires

Aluminium Wall

Major accomplishments in FY14

- Compared water treatment system module cost prediction with engineering based model.
- WTM ready to be released for public use
- Developed and linked ROM for brine production to CO_2-PENS
- Numerical simulations of homogenous and heterogeneous column experiment results
- Developed ROM for determining CO_2 storage potential during CO_2-EOR operations
- Initiated study on characterizing multi-phase CO_2-brine flow through faults
- 2 Peer-reviewed journal publications, 2 journal articles under review, 3 journal articles under preparation (to be submitted to IJGGC)
- Multiple presentations at 2013 Fall AGU (3), 2014 CCUS Meeting (4), IEAGHG Joint Network Meeting
- Four presentations at GHGT-12

Future Plans

- System model for CO_2-EOR
  - Verify ROM predictions against field reported data
  - Integrate ROM with CO_2-PENS and develop related capabilities in CO_2-PENS
- Complete 2-D tank experiments on shallow aquifer multi-phase flow characterization and numerical models
- Extend fault flow characterization study to include fault complexities

Appendix

Organization Chart

- Project team
  - PI: Rajesh Pawar
  - Program Manager: Melissa Fox
  - Team Members:
    - Jeri Sullivan: Water treatment system modeling
    - Shaoping Chu: Water treatment system modeling
    - Prof. Tissa Illangasekare (Colorado School of Mines): CO_2 release experimental characterization
    - Michael Plampin (Colorado School of Mines): CO_2 release experimental characterization
    - Mike Porter: Numerical simulation of CO_2 release experiments
    - Elizabeth Keating: Fault flow characterization
    - Jennifer Wilson: Fault flow characterization