Systems Modeling & Science for Geologic Sequestration

Project Number: LANL FE10-003 Task 3

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U.S. Department of Energy
National Energy Technology Laboratory
Strategic Center for Coal's
FY10 Carbon Sequestration Peer Review
February 8 – 12, 2010

Collaborators

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- Mark Porter (LANL)

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 (2011 TPP):
  - Develop technologies to demonstrate that 99 percent of injected CO_2 remains in the injection zones.
- 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

Technical Status

CO_2-PENS for predicting long-term performance of geologic sequestration reservoir

- CO_2-PENS (CO_2-Prediction of Engineered Natural Sites) is a modular, systems level model
  - Developed since 2005 with DOE funding.
  - Currently being applied in NRAP, SWRP, BSCSP, US-China Consortium.
- CO_2-PENS:
  - Developed for assessment of long-term performance of specific sites.
    - Provide input for various criteria: effectiveness (capacity & injectivity), HSE risks, economics, public policy
  - Supports a science based quantitative risk assessment.
  - System level approach that integrates modules that are governed by different physics and are described by analytical/semi-analytical/detailed numerical models.
  - Probabilistic predictions.
- Project Goals:
  - Develop capabilities in CO_2-PENS for assessing produced water treatment
  - Develop capabilities in CO_2-PENS for assessing CO_2 storage capacity in CO_2-EOR operations

Water Production & Treatment

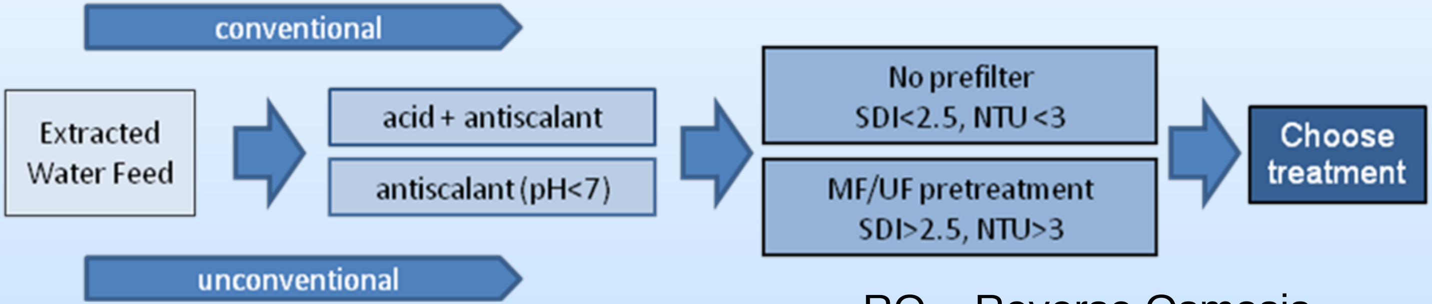
Water production and treatment for beneficial reuse

- 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.

Model Structure, Pretreatment and Treatment Choices

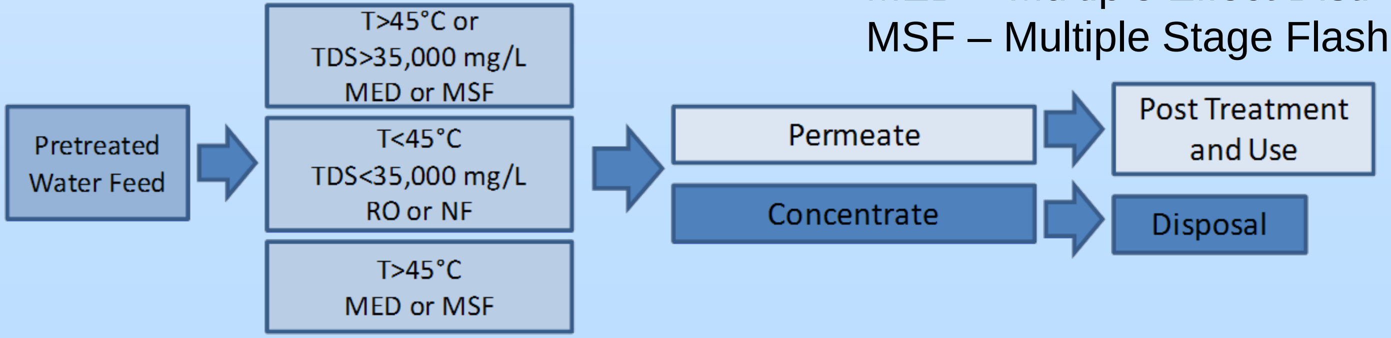
- Variable input pH, turbidity, temperature, salinity, desired output quality, treatment scenarios, energy recovery (pressure), feed volume (10 MGD or 37,854 m^3/d is standard scenario)
- RO passes restricted to maximum of 3, otherwise cycles and costs accumulate until desired treated % of feed is reached
- Model selects correct pretreatments, treatments to use and feasible concentrate disposal options

Pretreatment train



RO – Reverse Osmosis
NF – Nano Filtration
MED – Multiple Effect Distillation
MSF – Multiple Stage Flash

Treatment train



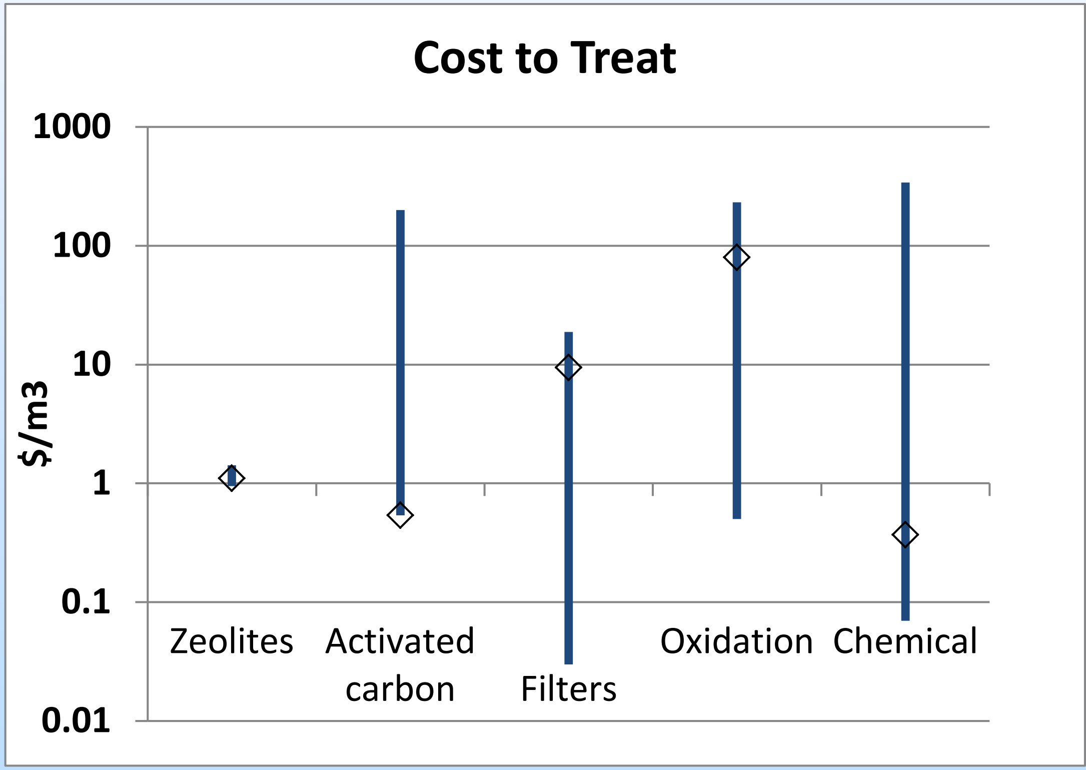
FY13 Tasks

- Extend applicability to CO_2-EOR related applications (organic pre-treatment)
- Incorporate costs associated with transportation

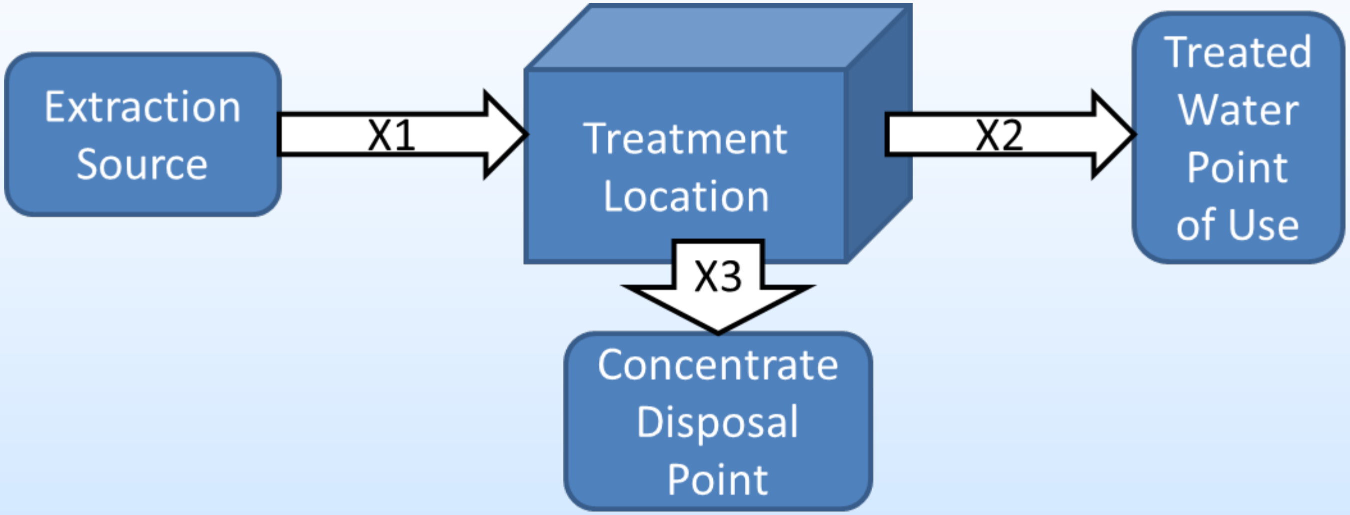
Organic pretreatment

- Organic pretreatments likely needed if EOR field utilized
  - May still be needed for other reservoirs (depleted oil and gas)
- Concentrations from sub-ppb to >10,000 mg/L; Free-phase oils or colloids

- *Organic pretreatment costs are highly variable in the literature*
  - Site-specific
  - Alberta reservoir listing: only if gas or oil is present
  - USGS PW database: out of date, variable data quality, no organic data

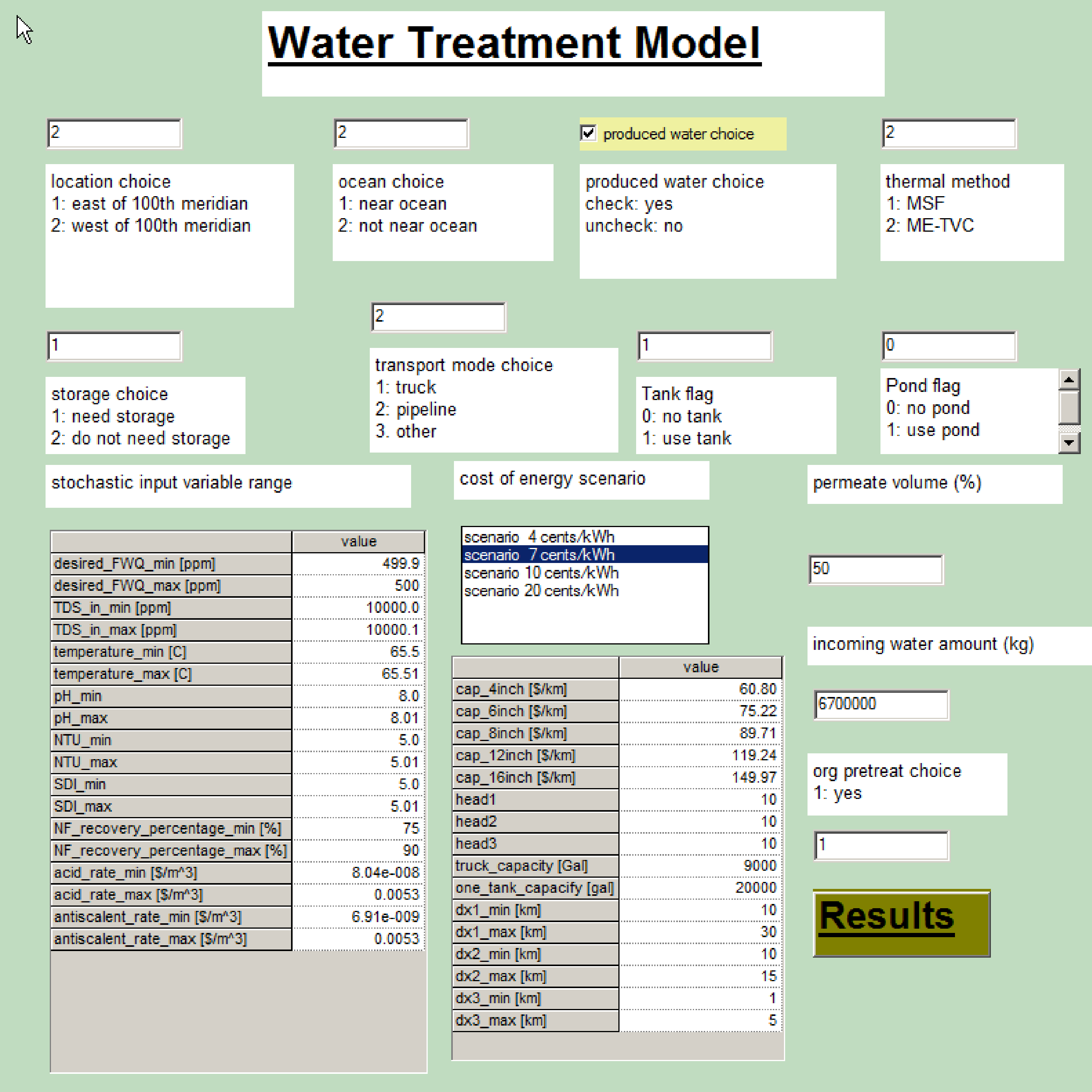


Simple Transport Model



X1 and X2- longest potential distances
X3 shortest (e.g., onsite disposal)
Trucking or Pipelines used
Pipeline capacity increases with volume as needed

Water Module Input Dashboard



2

location choice
1: east of 100th meridian
2: west of 100th meridian

2

ocean choice
1: near ocean
2: not near ocean

☑ produced water choice

produced water choice
check: yes
uncheck: no

2

thermal method
1: MSF
2: ME-TVC

1

storage choice
1: need storage
2: do not need storage

2

transport mode choice
1: truck
2: pipeline
3. other

1

Tank flag
0: no tank
1: use tank

0

Pond flag
0: no pond
1: use pond

stochastic input variable range

	value
desired_FWQ_min [ppm]	499.9
desired_FWQ_max [ppm]	500
TDS_in_min [ppm]	10000.0
TDS_in_max [ppm]	10000.1
temperature_min [C]	65.5
temperature_max [C]	65.51
pH_min	8.0
pH_max	8.01
NTU_min	5.0
NTU_max	5.01
SDI_min	5.0
SDI_max	5.01
NF_recovery_percentage_min [%]	75
NF_recovery_percentage_max [%]	90
acid_rate_min [$/m^3]	8.04e-008
acid_rate_max [$/m^3]	0.0053
antiscalent_rate_min [$/m^3]	6.91e-009
antiscalent_rate_max [$/m^3]	0.0053

cost of energy scenario

scenario 4 cents/kWh
scenario 7 cents/kWh
scenario 10 cents/kWh
scenario 20 cents/kWh

	value
cap_4inch [$/km]	60.80
cap_6inch [$/km]	75.22
cap_8inch [$/km]	89.71
cap_12inch [$/km]	119.24
cap_16inch [$/km]	149.97
head1	10
head2	10
head3	10
truck_capacity [Gal]	9000
one_tank_capacify [gal]	20000
dx1_min [km]	10
dx1_max [km]	30
dx2_min [km]	10
dx2_max [km]	15
dx3_min [km]	1
dx3_max [km]	5

permeate volume (%)

50

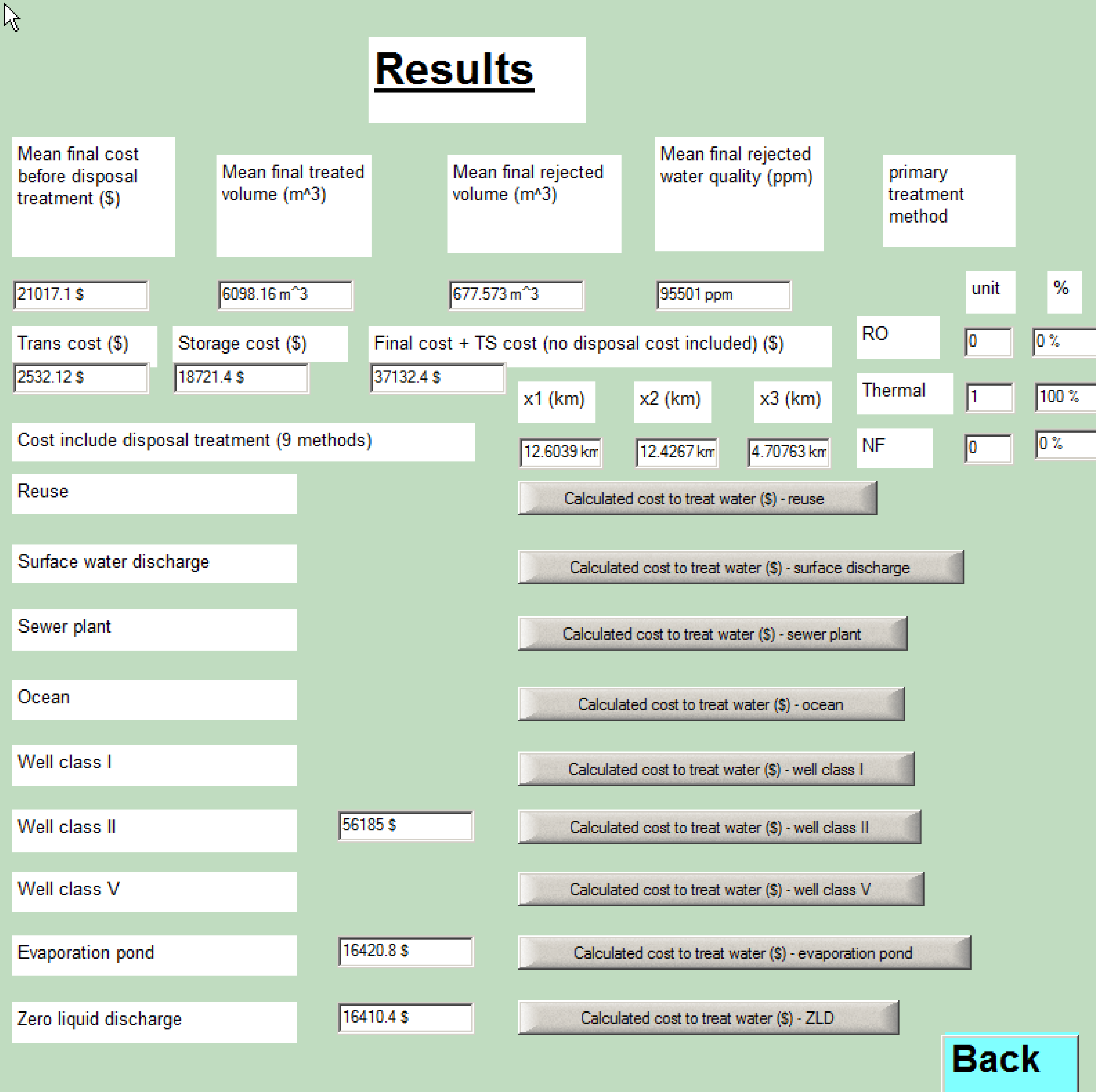
incoming water amount (kg)

6700000

org pretreat choice
1: yes

1

Water Module Output Dashboard



Results

Mean final cost before disposal treatment ($)	Mean final treated volume (m^3)	Mean final rejected volume (m^3)	Mean final rejected water quality (ppm)
21017.1 $	6098.16 m^3	677.573 m^3	95501 ppm

primary treatment method	unit	%
RO	0	0 %
Thermal	1	100 %
NF	0	0 %

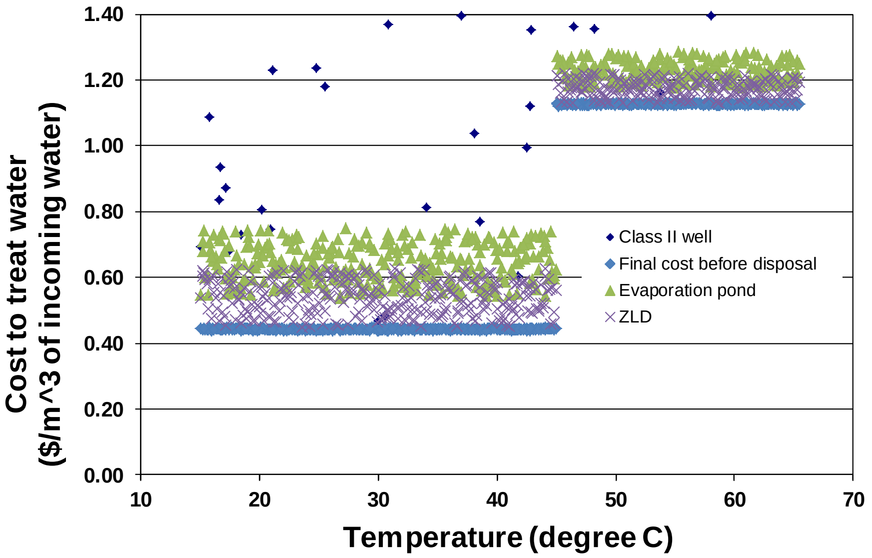
Trans cost ($)	Storage cost ($)	Final cost + TS cost (no disposal cost included) ($)
2532.12 $	18721.4 $	37132.4 $

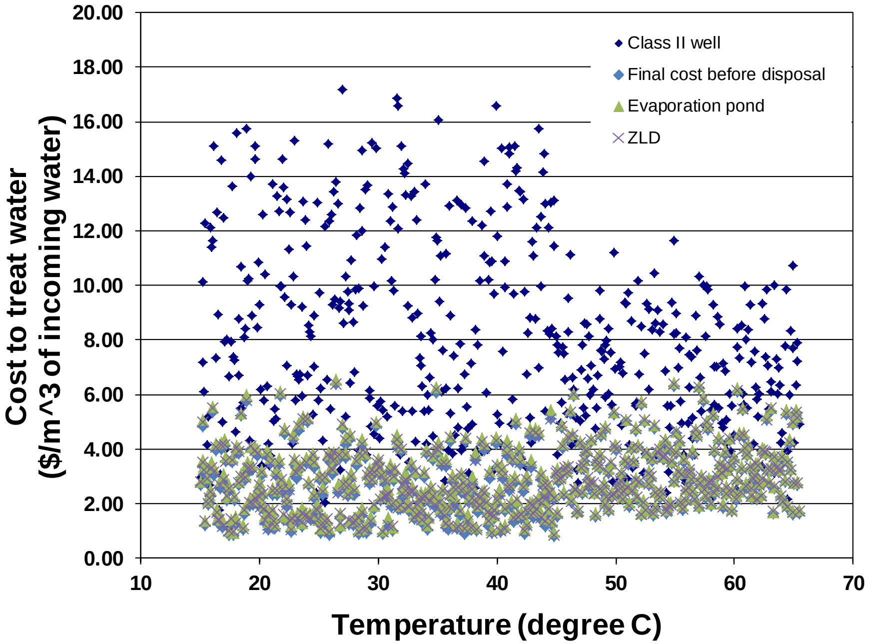
x1 (km)	x2 (km)	x3 (km)
12.6039 km	12.4267 km	4.70763 km

Cost include disposal treatment (9 methods)

Reuse	
Surface water discharge	
Sewer plant	
Ocean	
Well class I	
Well class II	56185 $
Well class V	
Evaporation pond	16420.8 $
Zero liquid discharge	16410.4 $

Example Application to Teapot Dome





Base case: Teapot Dome[1]

Q=6700 m3/d

T=15-65°C

RO, MED thermal methods

TDS=10,000 mg/L

Energy=$0.07 kWh

Permeate=50% of feed

500 realizations

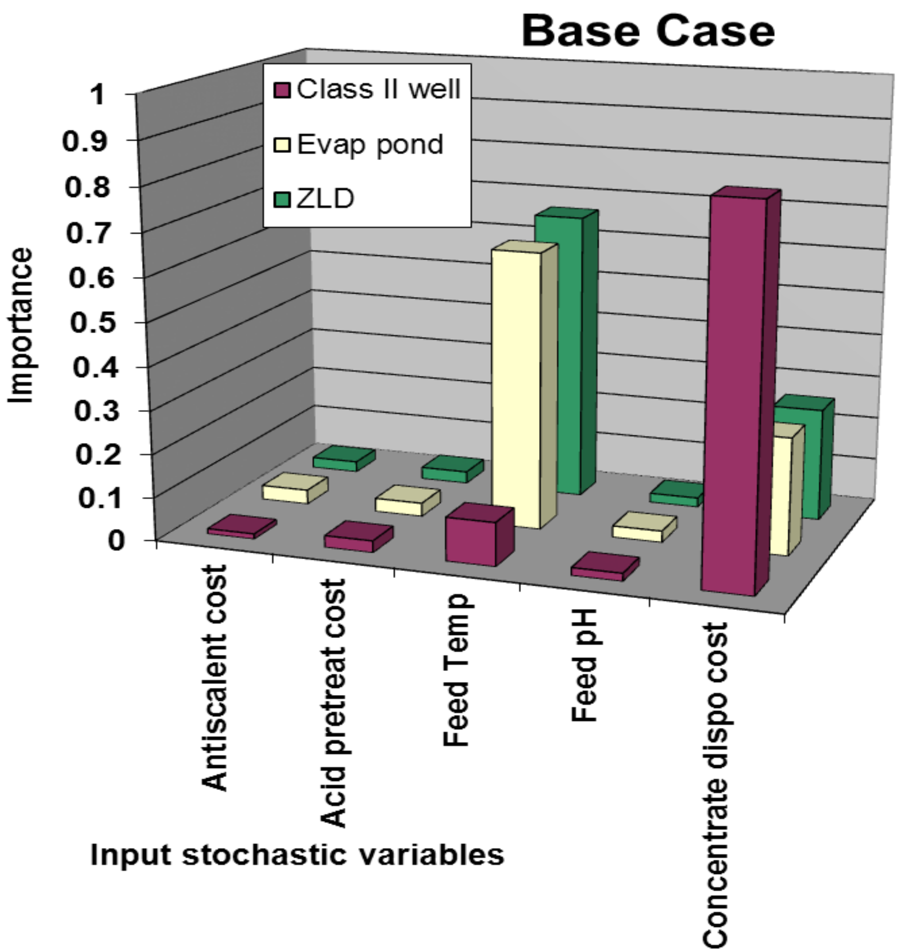
No transportation included

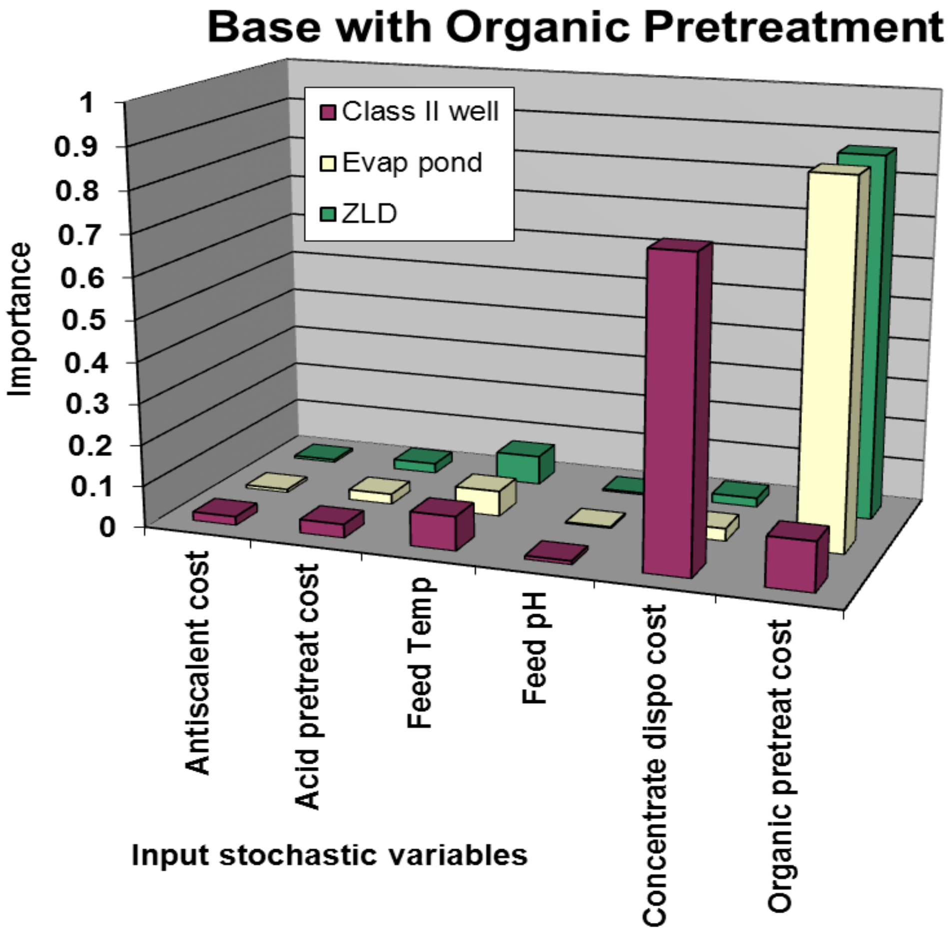
- Low-constraint organic pretreatment adds a large cost spread.
- Base spread is from various concentrate disposal methods

[1] Klapperich et al. 2012.

Importance Analysis

Disposal cost rates and feed water temperature become less important when organic pretreatment costs are included (except Class II well)


Base Case


Base with Organic Pretreatment

Next Steps

- Apply model to other site-specific data
- Link the water module to CO2-PENS
- Stand-alone model to be made publicly available

Long term CO_2 storage during EOR operations

Long term CO_2 storage during CO_2-EOR operations

- CO_2-EOR is a technology with dual benefits: potential long-term CO_2 storage with short-term economic incentives
  - Promote deployment of CCS in absence of a carbon policy driver
- Need to assess ultimate CO_2 storage potential:
  - For range of geologic/thermodynamic parameters and operational configurations
  - Potential oil recovery
- Goal: Develop a system module that can be used to calculate amount of CO_2 stored and oil recovered in CO_2-EOR operations
  - Quick calculations
  - Stochastic approach: Variable input parameters

Approach

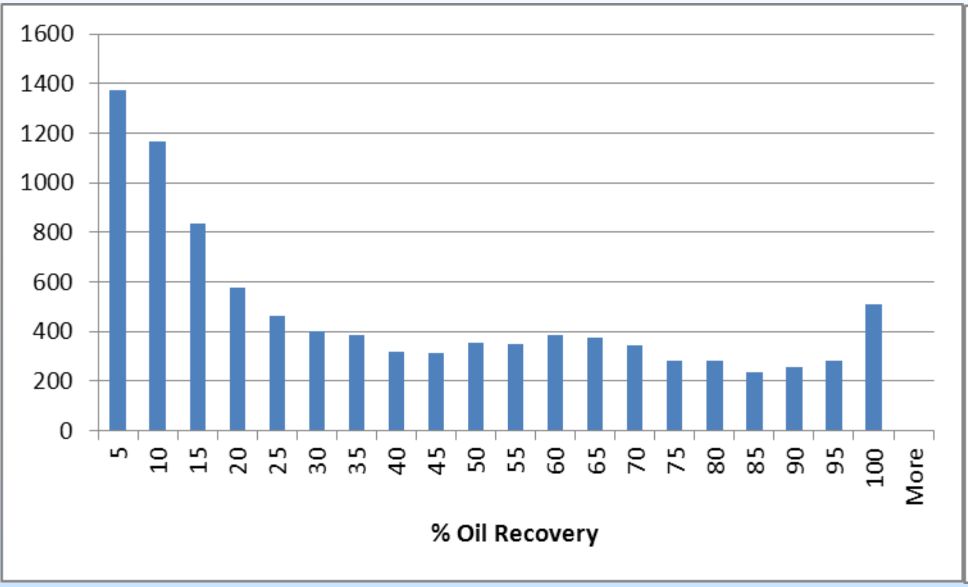
- Performed a set of compositional reservoir simulations to model CO_2 injection and resulting oil/gas recovery
  - Fully compositional model: account for thermodynamic interactions (CO_2 & in-situ hydrocarbons)
  - Range of geologic parameters: porosity, permeability, thickness
  - Heterogeneous porosity & permeability distributions using geostatistical approach
  - Range of thermodynamic/fluid parameters: oil compositions, relative permeability curves, reservoir temperature, reservoir pressure
  - Range of operational parameters: CO_2 injection time, maximum reservoir pressure
  - Geologic data (Takacs et al., 2010), Thermodynamic data (Haeberle, 2004)
- Compositional reservoir simulator: SENSOR6k
  - Quarter spot calculation with a single injector and single producer
- Monte-Carlo simulations using Latin Hyper Cube sampling approach: 10000 simulations

Parameter Ranges

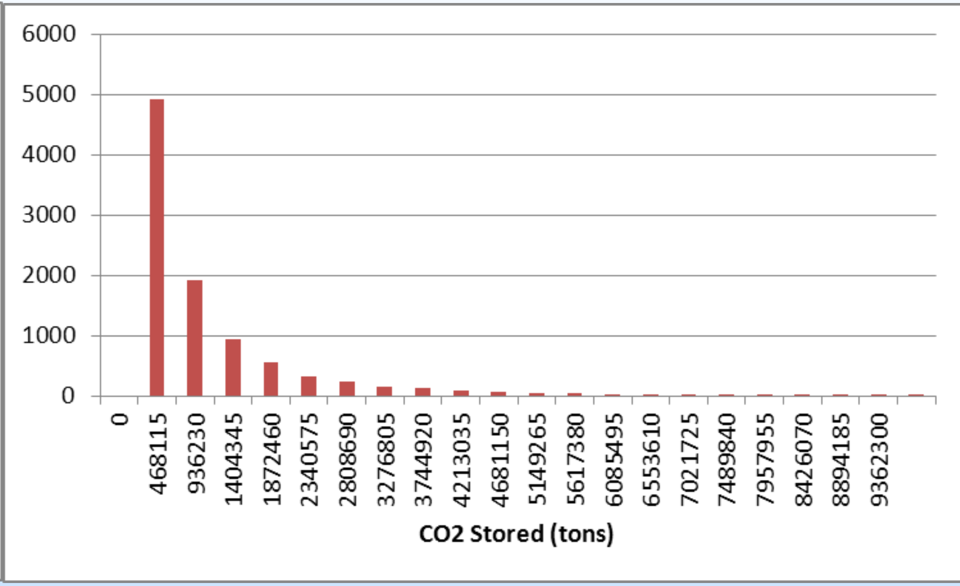
Parameter	**Minimum**	**Maximum**
Porosity	0.05	0.3
Average Permeability (md)	1	10
Thickness (ft)	50	800
Time (years)	5	50
Pmax (psi)	800	6400
Temperature (degrees F)	80	250
Mole Fractions for C1, C3-C5, C6, C10, C21, C36	0	1

Simulation Results

Histogram of % Oil Recovery

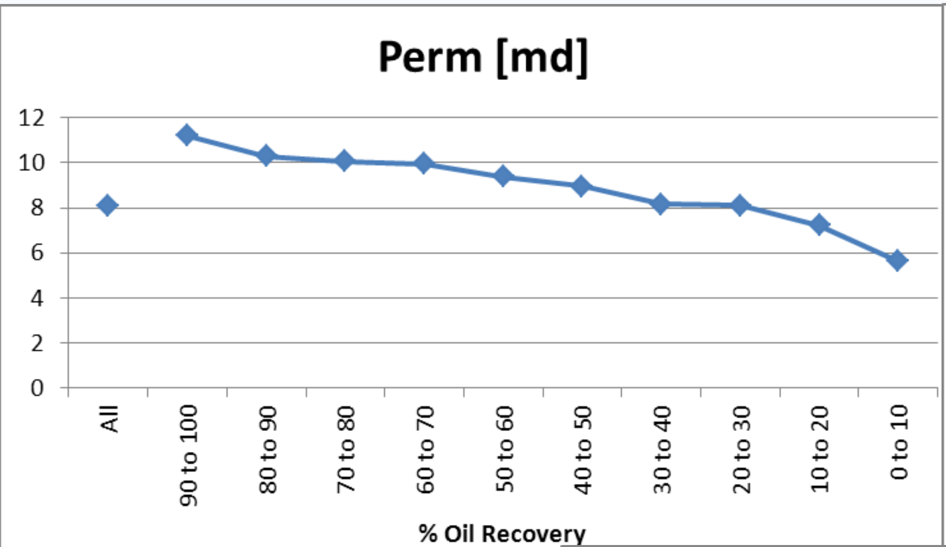


Histogram of Amount of CO_2 Stored

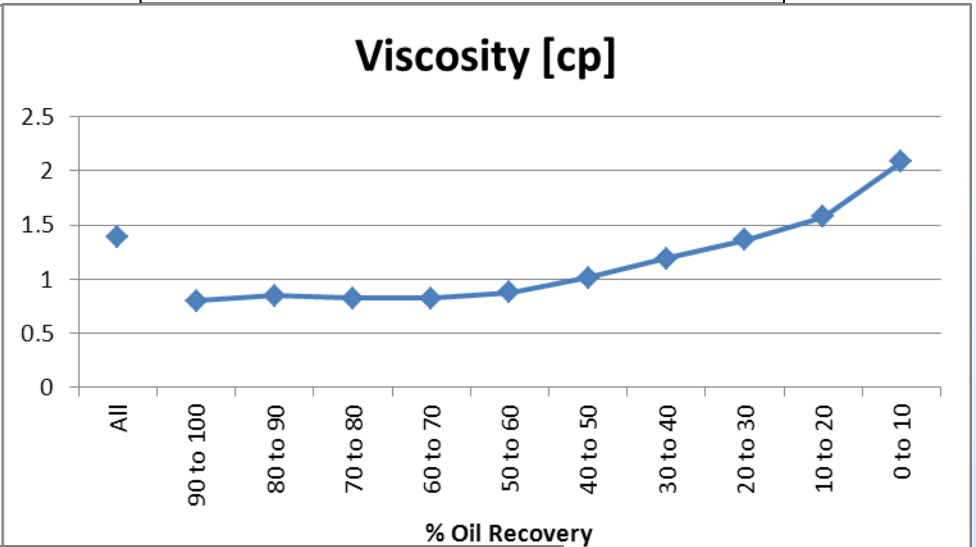


Effects of Parameters

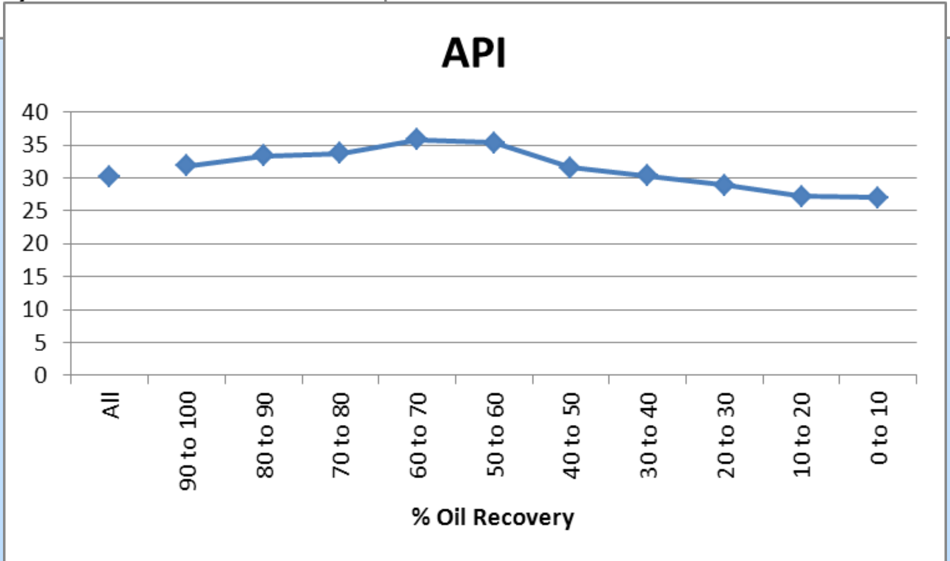
Permeability (avg.) on % Oil Recovery



Viscosity on % Oil Recovery



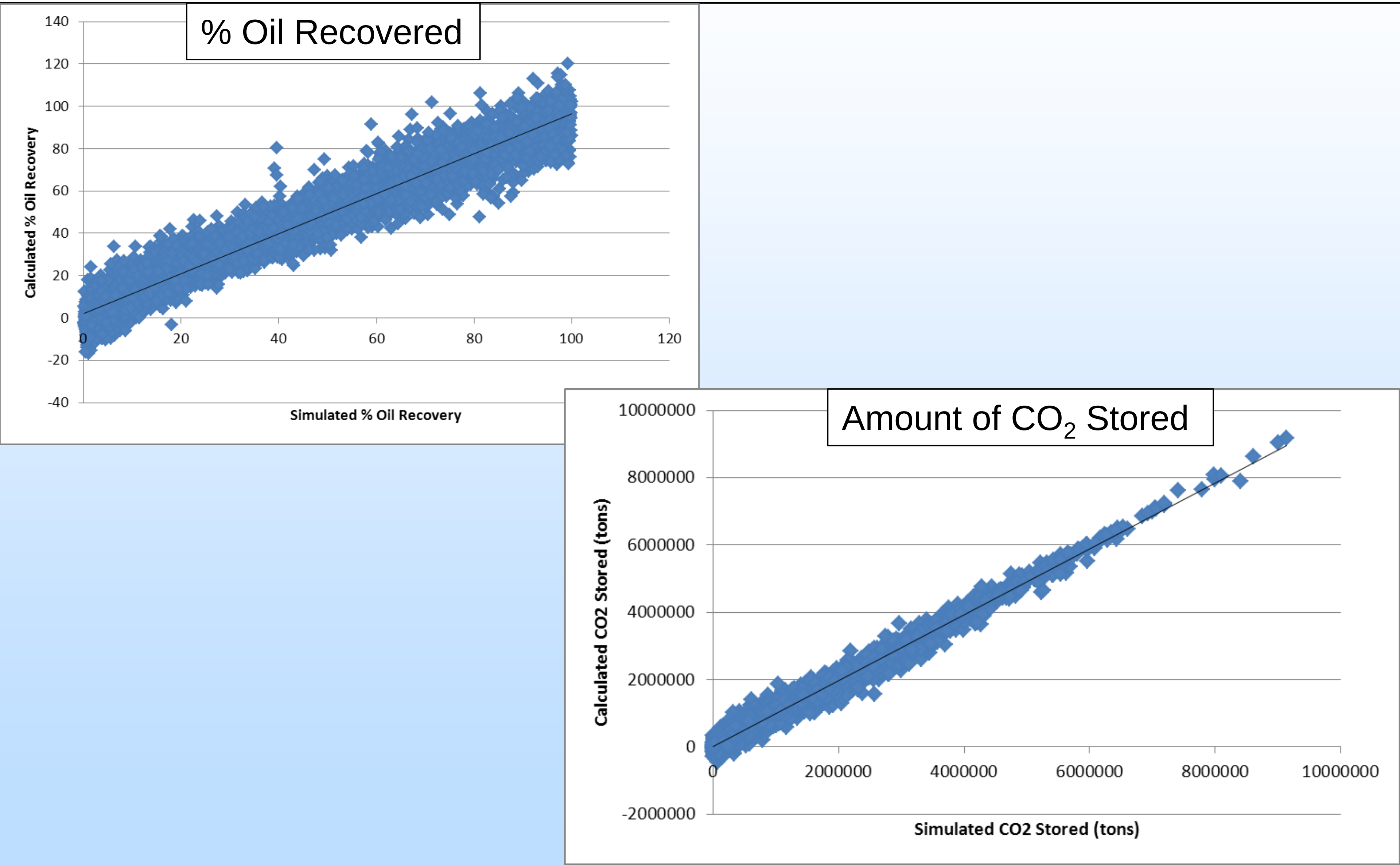
API on % Oil Recovery



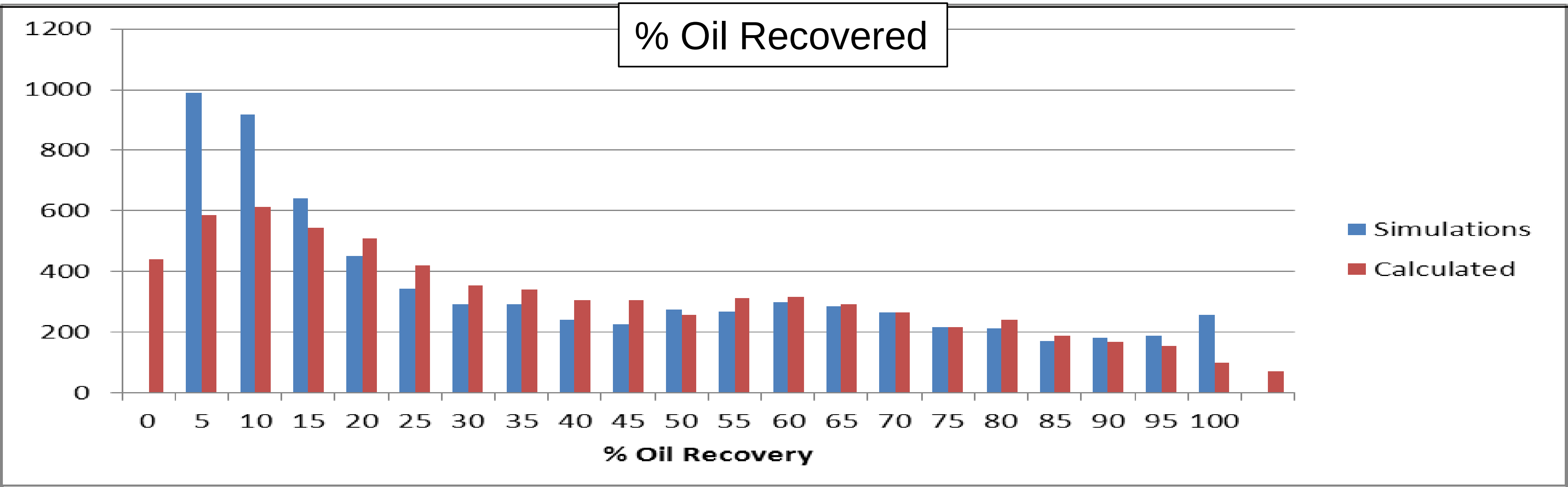
Reduced Order Model

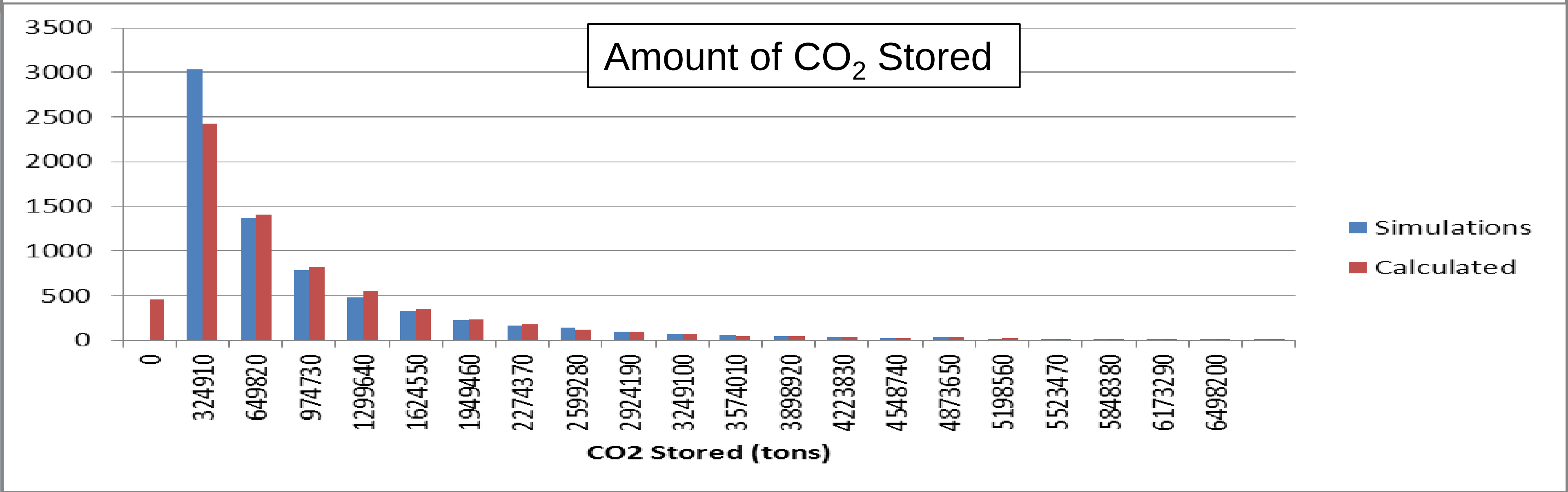
- Compositional simulation results used to develop a reduced order model (ROM)
  - % oil recovered and amount of CO_2 stored as a function of uncertain input parameters
  - MARS (Multi-variate Adaptive Regression Spline) approach

Comparison of calculated values against predictions of ROM



Comparison of calculated values against predictions of ROM


% Oil Recovered


Amount of CO_2 Stored

Next Steps

- Develop ROMs for other types of EOR field operations: different patterns (e.g.) line drive, different flooding approaches (WAG)
- Verify ROMs predictions against field reported data
- Integrate ROM with CO_2-PENS and develop related capabilities in CO_2-PENS

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
- 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-FY13:
  - Completed long 1D column experiments (4m)
  - 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.
- FY13:
  - Performed multiple short (1.36m) 1D & pseudo-2D column experiments focused on characterizing effect of heterogeneity.
  - Numerical simulation of column experiments.

Short 1D column experiments for testing effect of heterogeneity on gas phase evolution

- Understand:
  - How geologic heterogeneity enhances CO_2 gas evolution and whether this effect can be quantified
    - Using a measure of “oversaturation pressure”
  - What are the limits on sand contrasts which lead to gas phase evolution
  - How do different types of sand interfaces (finer-over-coarser, coarser-over-finer) affect gas phase evolution

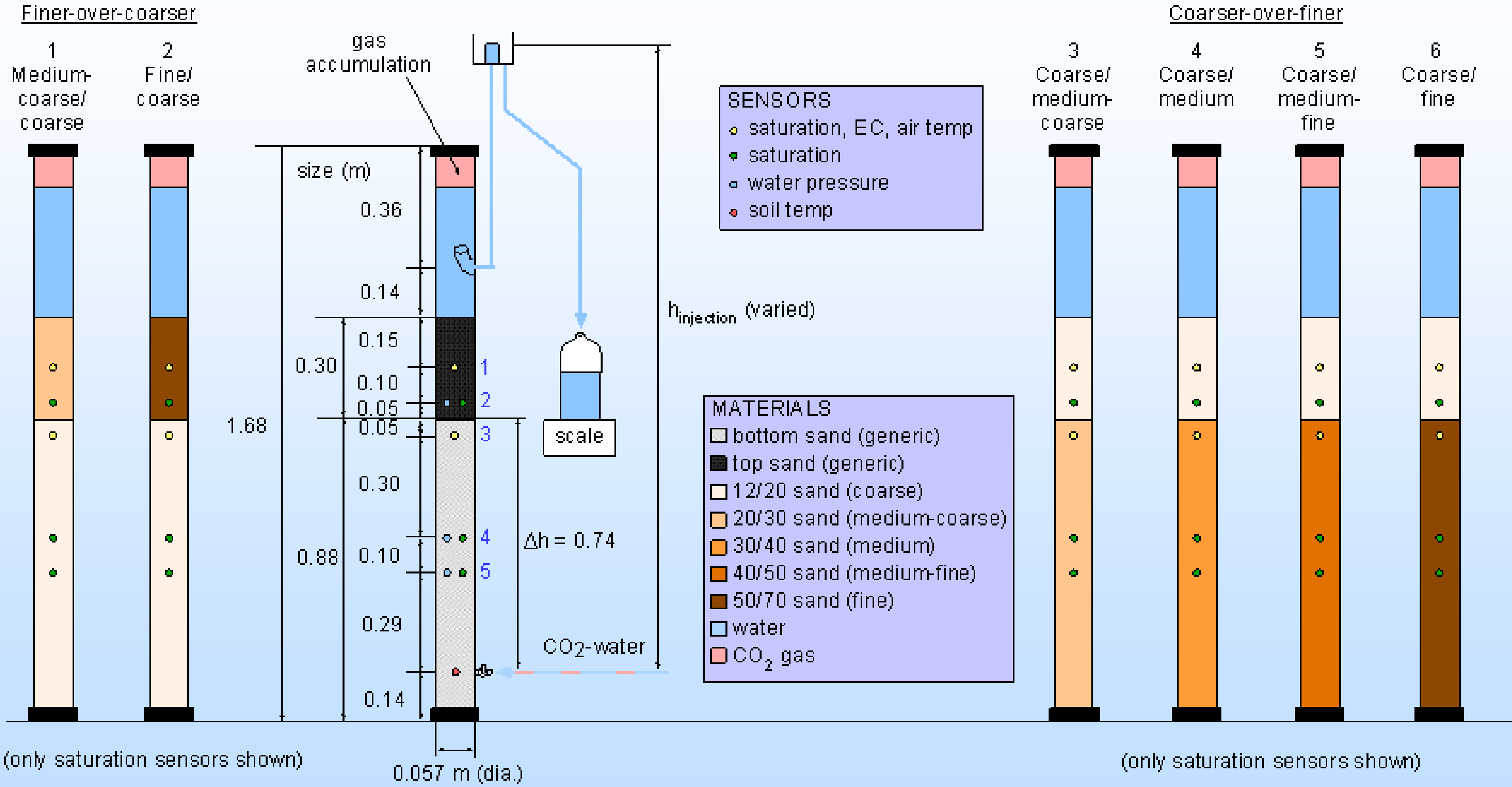
Measure for degree of oversaturation

Over saturation pressure defined as $\Delta P_{os} = \Delta P_{inj} + \Delta P_e$ may control gas phase evolution

ΔP_{inj}: Difference in the saturation pressure and hydrostatic pressure, ΔP_e: Difference in the gas entry pressure for two sands at the heterogeneity interface

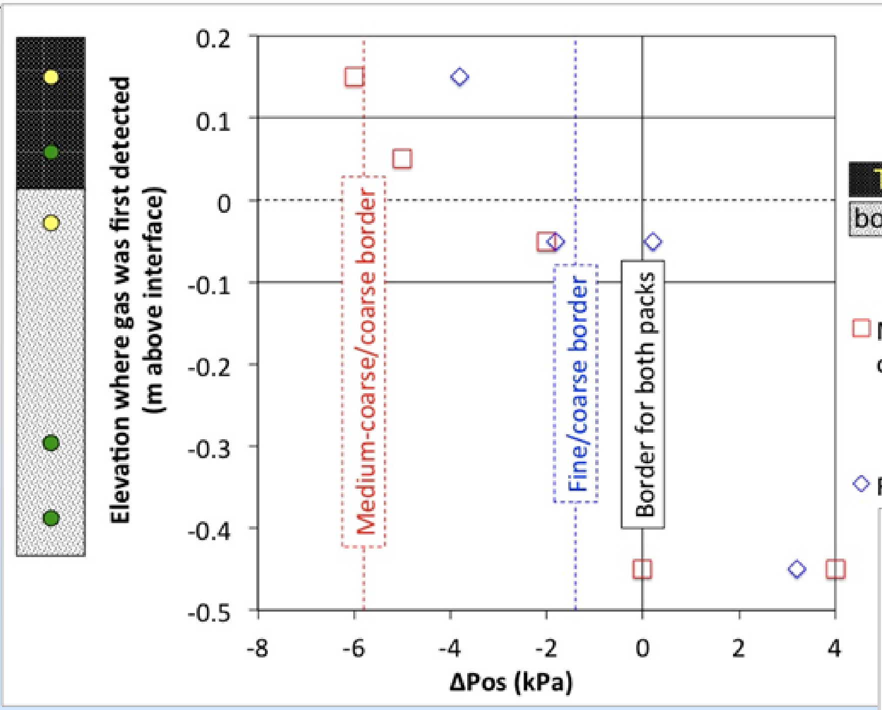
ΔP_{os}**≥0**	Gas phase should evolve at the bottom of column, irrespective of heterogeneity
$\Delta P_{os} < \Delta P_{os,min}$ $\Delta P_{os,min} = 2P_{e,top\ sand} - P_{e,bottom\ sand} - \rho g \Delta h$	Gas phase will not evolve near the heterogeneity interface, the presence of heterogeneity does not have an effect on gas phase evolution

Column experiments to characterize effect of heterogeneity



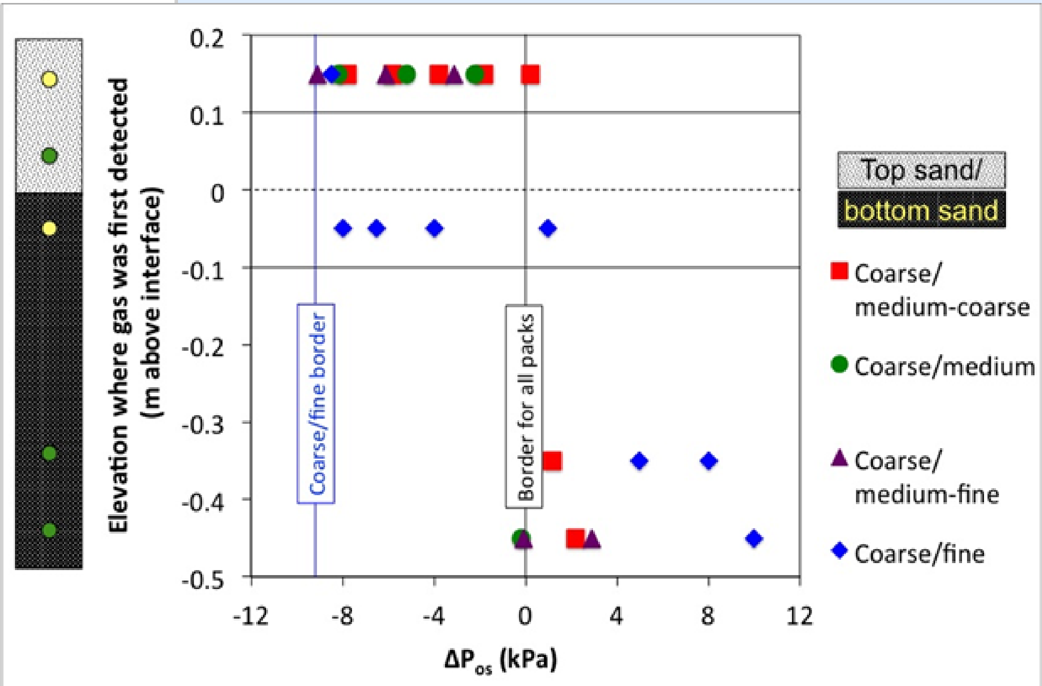
Performed 35 different experiments: multiple injection pressures for each packing configurations

Results of 1-D column experiments to characterize effect of heterogeneity

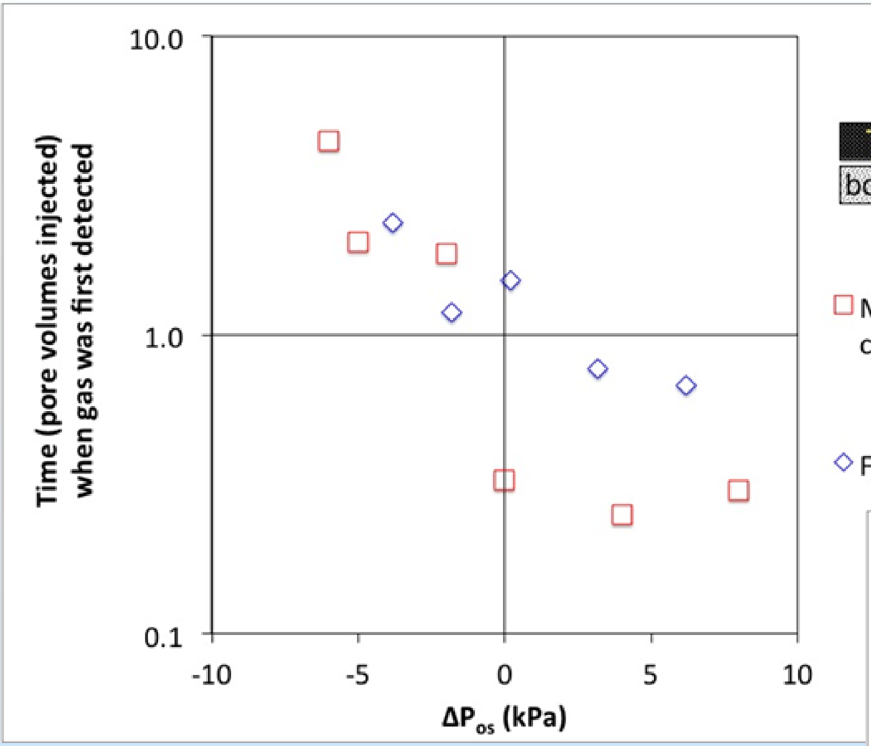


- Gas phase was first detected near the bottom of the column for $\Delta P_{os} > 0$ kPa
- Gas phase was first detected near the top of the column when $\Delta P_{os} < \Delta P_{os,min}$

- For three packing configurations gas phase was detected near heterogeneity interface
- Finer over coarse have more effect on gas phase evolution unlike coarse over fine unless the sand size contrast is high

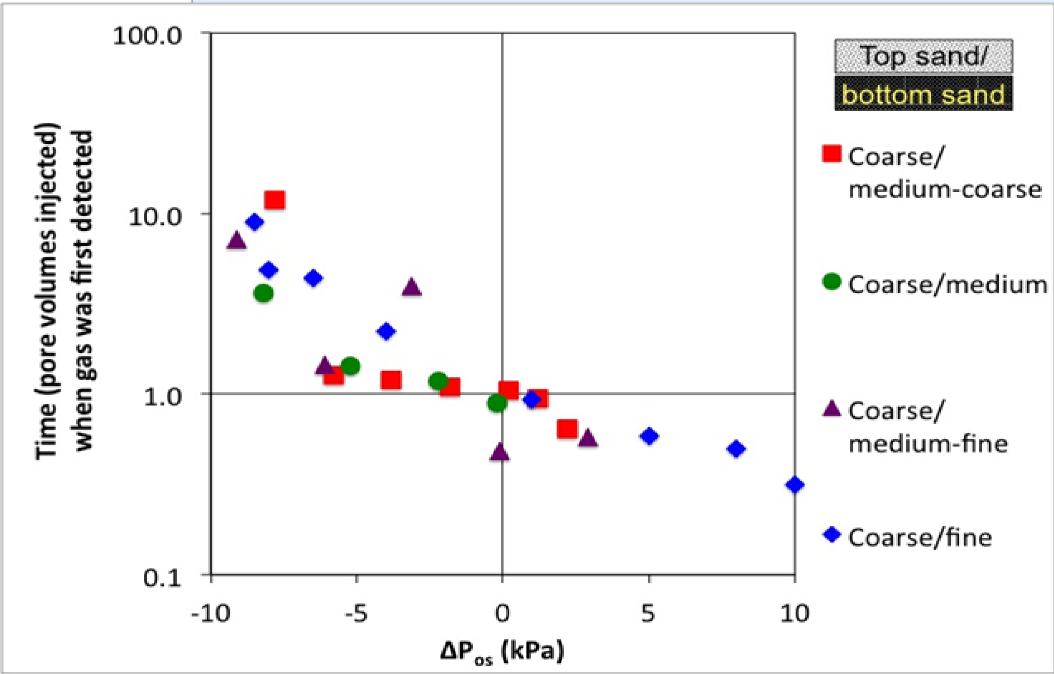


Results of 1-D column experiments to characterize effect of heterogeneity

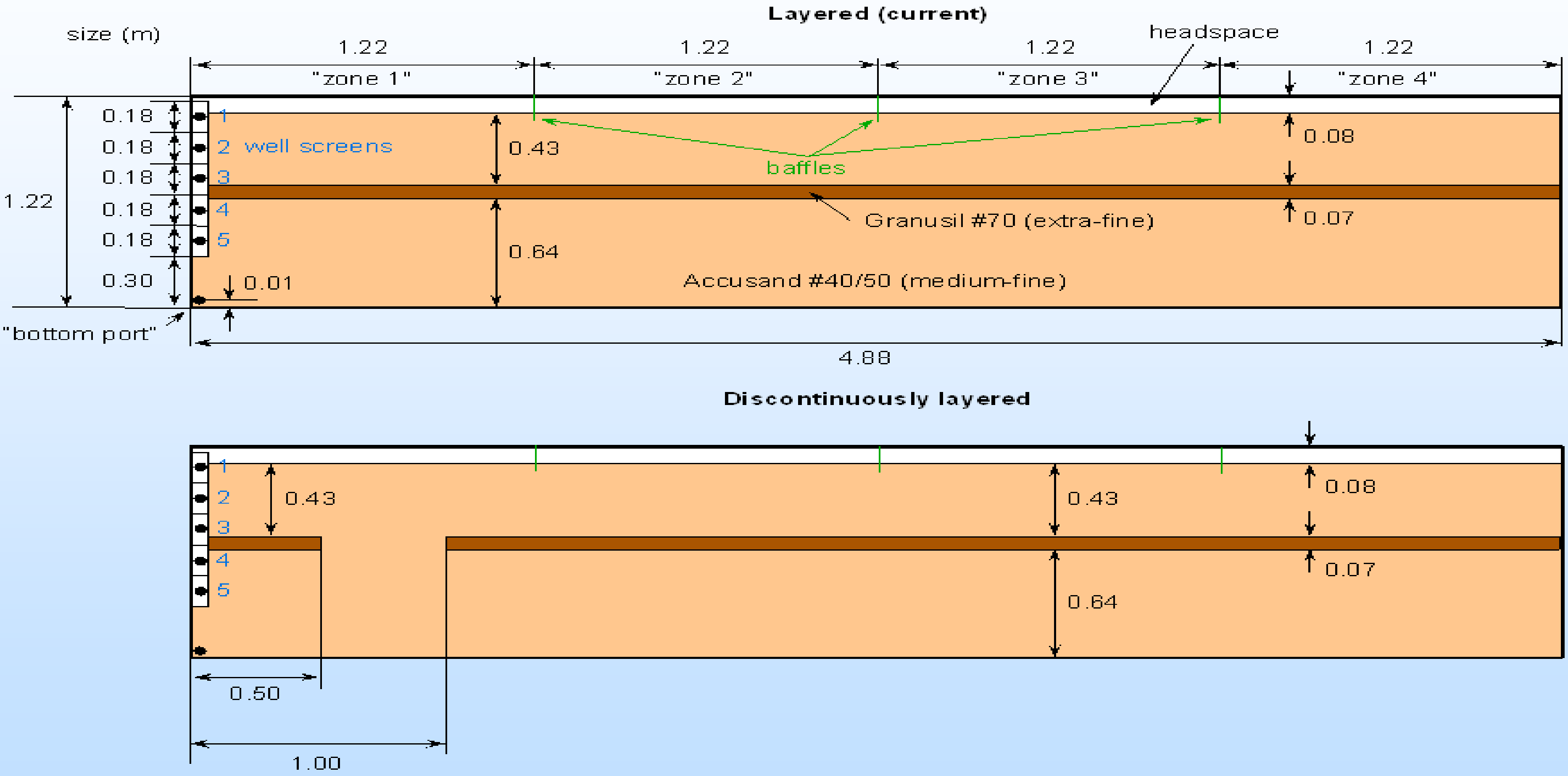


- Gas phase evolved *before* one pore volume had been injected when ΔP_{os} > 0 kPa, and *after* one pore volume had been injected when ΔP_{os} < 0 kPa.

- Gas phase evolution delayed for heterogeneous sands with larger contrasts.



Future work: 2-D tank experiments to characterize effect of heterogeneity



Major accomplishments in FY13

- Developed a comprehensive systems module for water production to minimize risks and treatment for beneficial reuse.
- Developed a multi-parameter reduced order model to efficiently compute amount of CO_2 stored and oil recovered during CO_2-EOR operations
- Completed short 1D and pseudo 2D column experiments to characterize effect of heterogeneity on multi-phase evolution and flow subsequent to CO_2-water leakage
  - Experimental observations are filling-in knowledge base on multi-phase (CO_2-water) evolution in shallow aquifer.
- 1 Peer-reviewed journal publication, 1 journal article under review, 1 journal article under preparation
- Presentations at 2012 Fall AGU, 2013 CCUS Meeting

Future Plans

- System model for CO_2-EOR
  - Develop ROM for other types of EOR field operations: line drive, WAG
  - Verify ROM predictions against field reported data
  - Integrate ROM with CO_2-PENS and develop related capabilities in CO_2-PENS
- System model for water treatment:
  - Apply model to other site-specific data
  - Link the water module to CO_2-PENS
  - Stand-alone model to be made publicly available
- Complete 2-D tank experiments on shallow aquifer multi-phase flow characterization and numerical models

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
    - Jacob Bauman: CO2-EOR/Sequestration ROM deveopment
    - 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

Publications and presentations

Publications:

- Sakaki, T., Plampin, M.R., et al., 2013. What controls carbon dioxide exsolution in the subsurface? ~Experimental observations in a 4.5m-long column under different heterogeneity conditions (in press). *International Journal of Greenhouse Gas Control*, 13
- Plampin, M., Sakaki, T., Illangasekare, T., and Pawar, R., An Intermediate-Scale Experimental Investigation into the Effects of Heterogeneity on CO_2 Gas Phase Evolution in Shallow Subsurface Environments During Leakage from Geologic Sequestration Sites, In review International Journal of Greenhouse Gas Control
- Sullivan, E. J., Chu, S., Stauffer, P., Pawar, R., A CO_2-PENS model of methods and costs for treatment of water extracted during geologic carbon sequestration, in-press, Desalination and Water Treatment Journal
- Sullivan, E. J., Chu, S., Stauffer, P., Middleton, R., Pawar, R., A method and cost model for treatment of water extracted during geologic CO_2 sequestration, in review, International Journal of Greenhouse Gas Control
- Middleton, R. S.; Keating, G. N.; Stauffer, P. H.; Jordan, A. B.; Viswanathan, H. S.; Kang, Q. J.; Carey, J. W.; Mulkey, M. L.; Sullivan, E. J.; Chu, S. P.; Esposito, R.; Meckel, T. A., The cross-scale science of CO_2 capture and storage: from pore scale to regional scale. *Energy & Environmental Science* 2012, *5*, (6), 7328-7345.
- Middleton, R. S.; Keating, G. N.; Stauffer, P. H.; Viswanathan, H. S.; Pawar, R. J., Effects of geologic reservoir uncertainty on CCS infrastructure. *International Journal of Greenhouse Gas Control* 2012, *8*, 132-142.
- Middleton, R. S.; Kuby, M. J.; Bielicki, J. M., Generating candidate networks for optimization: The CO_2 capture and storage optimization problem. *Computers, Environment and Urban Systems* 2012, *36*, (1), 18-29.
- Middleton, R. S.; Wei, R.; Kuby, M. J.; Keating, G. N.; Pawar, R. J., A dynamic model for optimally phasing in CCS infrastructure. *Environmental Modeling and Software* 2012 37, 195-203.
- Keating, G. N.; Middleton, R. S.; Stauffer, P. H.; Viswanathan, H. S.; Letellier, B. C.; Pasqualini, D.; Pawar, R. J.; Wolfsberg, A. V., Mesoscale Carbon Sequestration Site Screening and CCS Infrastructure Analysis. *Environmental Science & Technology* 2011, *45*, 215-222.
- Keating, G. N.; Middleton, R. S.; Viswanathan, H. S.; Stauffer, P. H.; Pawar, R. J., How storage uncertainty will drive CCS infrastructure. *Energy Procedia* 2011, *4*, 2393-2400.

Publications and presentations

Publications:

- Kuby, M. J.; Bielicki, J. M.; Middleton, R. S., Optimal Spatial Deployment of CO_2 Capture and Storage Given a Price on Carbon. *International Regional Science Review* 2011, *34*, (3), 285-305.
- Kuby, M. J.; Middleton, R. S.; Bielicki, J. M., Analysis of cost savings from networking pipelines in CCS infrastructure systems *Energy Procedia* 2011, *4*, 2808-2815.
- Middleton, R. S.; Bielicki, J. M.; Keating, G., N.; Pawar, R. J., Jumpstarting CCS using refinery CO_2 for enhanced oil recovery. *Energy Procedia* 2011, *4*, 2185-2191.
- Stauffer, P. H.; Keating, G. N.; Middleton, R. S.; Viswanathan, H. S.; Berchtod, K. A.; Singh, R. P.; Pawar, R. J.; Mancino, A., Greening Coal: Breakthroughs and Challenges in Carbon Capture and Storage. *Environmental Science & Technology* 2011, *45*, (20), 8597-8604

Publications and presentations (continued)

Presentations:

Sullivan, J., Chu, S., Pawar, R., (2013) Impacts of treatment and transportation choices on the cost profile of water extracted during carbon storage, Twelveth Annual Conference on Carbon Capture, Utilization & Sequestration, Pittsburgh, PA.

Plampin, M., Illangasekare, T., Pawar, R., (2012) The Effects of Heterogeneity on CO_2 Gas Phase Evolution in the Shallow Subsurface During Leakage from Geologic Sequestration Sites: Intermediate Scale Experiments, Fall AGU meeting, San Francisco, CA.

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Middleton, R.S., Keating, G.N., Stauffer, P.H., Viswanathan, H.S., and Pawar, R.J. (2010). The impact of geologic reservoir uncertainty on CCS infrastructure, Ninth Annual Conference on Carbon Capture & Sequestration, Pittsburgh PA.

Publications and presentations (continued)

Presentations:

Sullivan, E.J., S. Chu, P. Stauffer and R. Pawar (2010). A system model of methods, processes, and costs for treatment of water produced during CO2 sequestration. 9th Annual Conference on Carbon Capture and Sequestration, Pittsburgh, PA.

Sullivan, E.J., S. Chu, P.H. Stauffer and R.J. Pawar (2010). Development of a system model of methods, processes and costs for treatment of water extracted during carbon sequestration, Energy Resources and Produced Water Conference, University of Wyoming, Laramie, WY..

Middleton, R. S.; (2010). Spatial energy infrastructure modeling: carbon capture and storage, George Mason University, Department of Geography and GeoInformation Science

Middleton, R. S. (2010). Energy development and climate change at the basin scale: the water-land-carbon nexus, Pacific Northwest Laboratory/University of Maryland, Joint Global Change Research Institute

Middleton, R. S.; (2010). Spatial energy infrastructure modeling: carbon capture and storage, Stanford University, Department of Energy Resources Engineering

We participate and collaborate regularly with the Water Working Group for the Partnerships. This group seeks to identify water issues related to CO_2 capture and storage, perform outreach education on these issues, and to disseminate water research performed within the Capture program and the Partnerships