Systems Modeling & Science for Geologic Sequestration

Project Number: LANL FE10-003 Task 3

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Presentation Outline

- Benefit to the program
- Project overview
- Project technical status
- Accomplishments to date
- Future Plans
- Appendix
  - Organization Chart
  - Gantt Chart
  - Bibliography

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Benefit to the program

- Program goals being addressed:
    - 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).

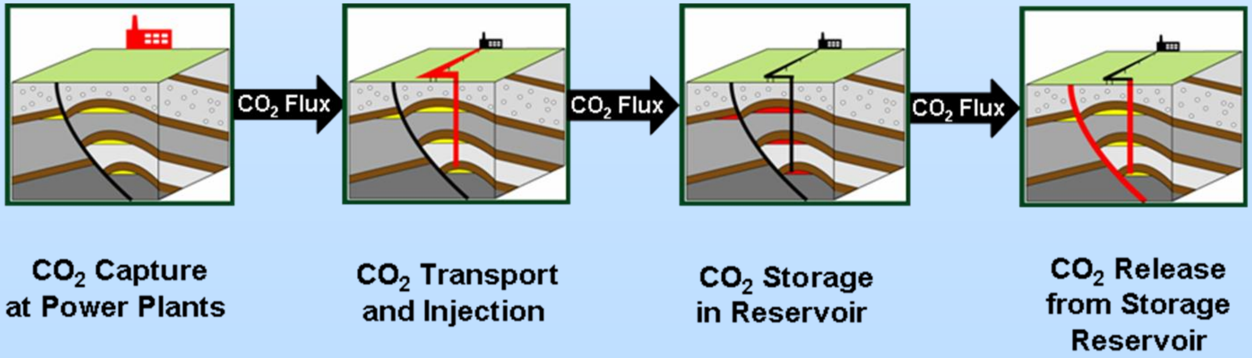
Project Overview:
Goals and Objectives

1. Develop and apply system modeling capabilities applicable to CCS storage operations:
    - Develop capabilities in LANL's CO_2-PENS system-model for a range of field site applications
    - Develop capabilities to assess optimized CCS infrastructure
    - Develop capabilities that can be used to evaluate water production and treatment for beneficial reuse.
2. Characterize multi-phase CO_2 flow in groundwater aquifers through an integrated experimental-simulation approach

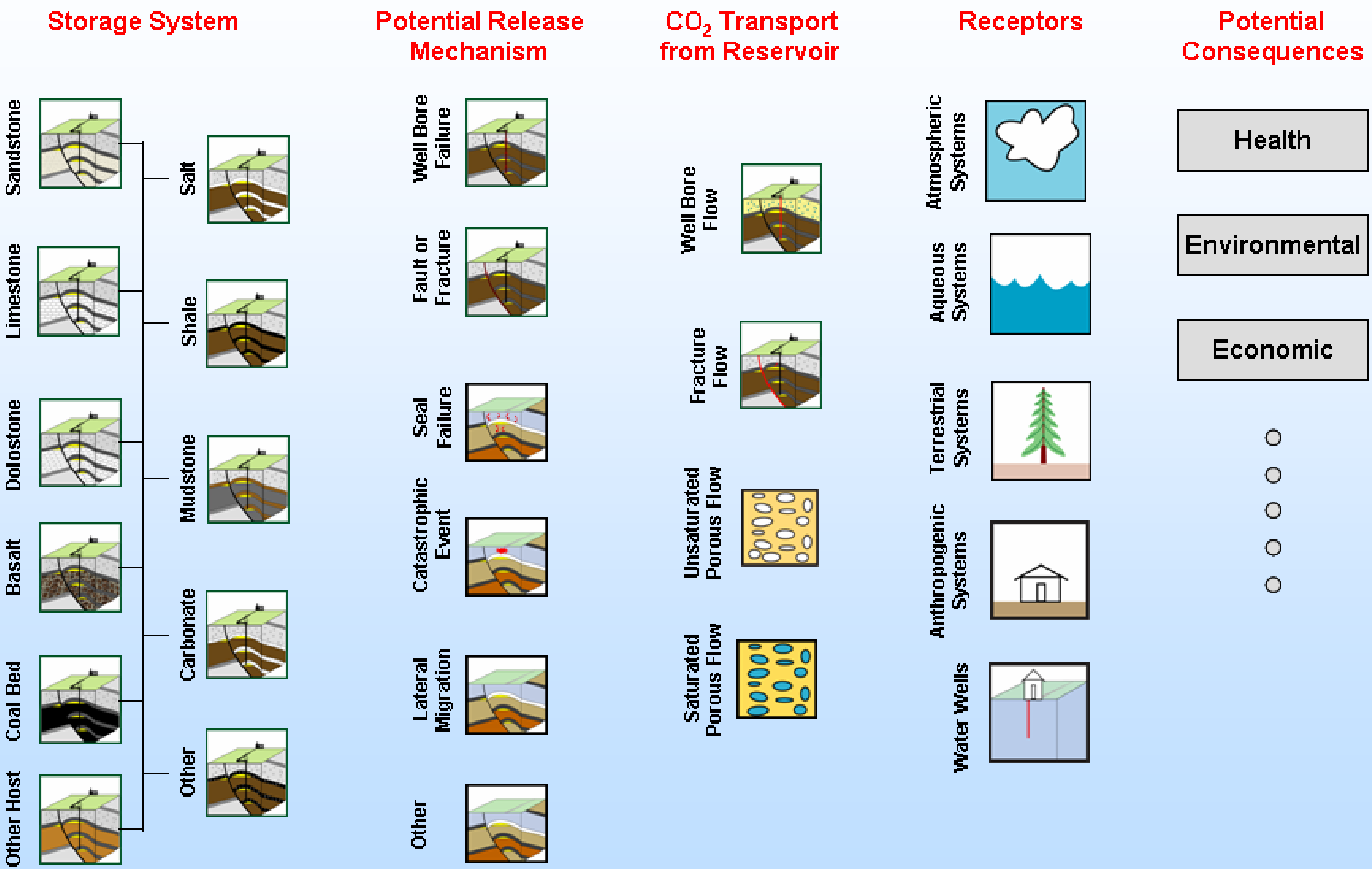
Technical Status

Developing an effective CCS technology deployment strategy for CO_2 management requires consideration of various coupled systems

- Components of the CCS technology, namely, CO_2 sources, transportation pipelines and storage reservoirs will interact and impact performance of each other
  - Suitable availability of geologic storage options and their long-term performance will influence siting, size and operations of power plants (or other CO_2 sources)
  - Infrastructure needed at a geologic storage site and effective site management will be influenced by the amount of CO_2 to be sequestered
  - Development of an efficient pipeline network will depend on the distribution of sources and storage sites
- Predicting the performance of the integrated CCS operation and assessing its effectiveness can be done with a system modeling approach



A system model for geologic storage encompasses all components at storage site



Storage System

- Sandstone
- Limestone
- Dolostone
- Basalt
- Coal Bed
- Other Host
- Salt
- Shale
- Mudstone
- Carbonate
- Other

Potential Release Mechanism

- Well Bore Failure
- Fault or Fracture
- Seal Failure
- Catastrophic Event
- Lateral Migration
- Other

CO_2 Transport from Reservoir

- Well Bore Flow
- Fracture Flow
- Unsaturated Porous Flow
- Saturated Porous Flow

Receptors

- Atmospheric Systems
- Aqueous Systems
- Terrestrial Systems
- Anthropogenic Systems
- Water Wells

Potential Consequences

- Health
- Environmental
- Economic

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At LANL we have developed the first-ever system level model, CO_2-PENS, for predicting long-term performance of a geologic sequestration reservoir

- CO_2-PENS (CO_2-Prediction of Engineered Natural Sites) is a modular, systems level model developed to perform comprehensive analysis of CO_2 sequestration sites
  - 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
  - Simulate CO_2 transport & migration from sources to storage & beyond.
  - 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.

Technical approach

- Integrate CO_2-PENS with LANL's *SimCCS* model for optimization of infrastructure deployment
  - Enhance *SimCCS* capabilities to address time-dependence, incorporation of uncertainty and risk
- Develop new capabilities in CO_2-PENS to enhance its applicability:
  - Evaluate water production, treatment for beneficial reuse and disposal to minimize risks due to pressure increase
  - New modules for application to CO_2-EOR sites
- Demonstrate applicability of CO_2-PENS through field applications
- Fill-in the knowledge gap related to underlying science base:
  - Current understanding of CO_2 exsolution and multi-phase fluid flow in shallow aquifers

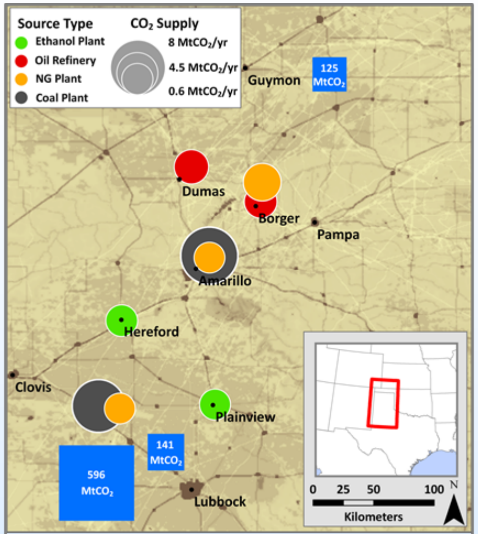
Optimization of CCS infrastructure deployment

- In order to develop an efficient and robust CCS infrastructure as the scale of CCS deployment grows we will have to *simultaneously* and *optimally decide*:
  - Which CO_2 sources will capture [or ***emit***] CO_2 and how much CO_2 to capture at selected sources
  - Which geological reservoirs to open, how much CO_2 to inject into each reservoir while taking into account CO_2 storage effectiveness
  - Where to construct pipeline *networks,* what diameter pipeline to build and how to efficiently distribute CO_2 amongst supply/demands

Optimization of CCS infrastructure deployment

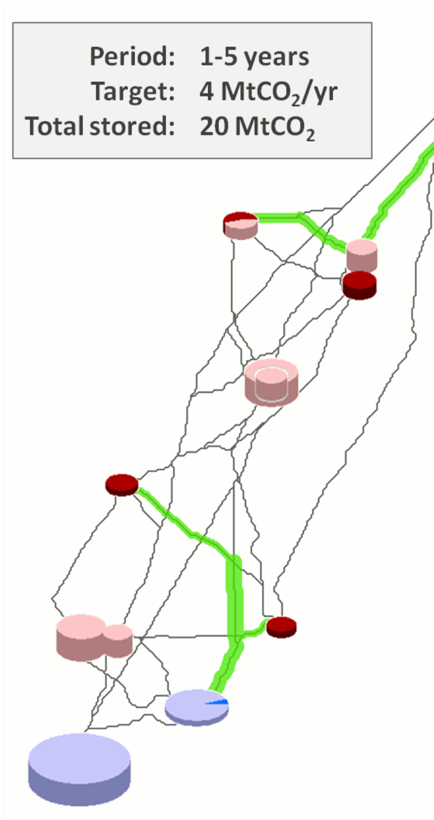
- An integrated modeling approach that while optimizing the transportation network it also takes into account the storage reservoir effectiveness
  - Our overall approach will be focused on integrating LANL's *SimCCS* optimization model with CO_2-PENS
    - ➢ *SimCCS* is a comprehensive CCS infrastructure model for optimization of CO_2 capture, transportation and storage: uses realistic, networked pipeline system
  - Use CO_2-PENS to inform *SimCCS*
    - ➢ CO_2-PENS provides information on number of wells, injectivity, maximum reservoir capacity, water production to maintain pressure at different sites
    - ➢ *SimCCS* updated to take into account reservoir related information
  - Use CCS infrastructure results to inform CO_2-PENS
    - ➢ Identify potential, feasible storage sites

Results: Spatial evolution of infrastructure over time

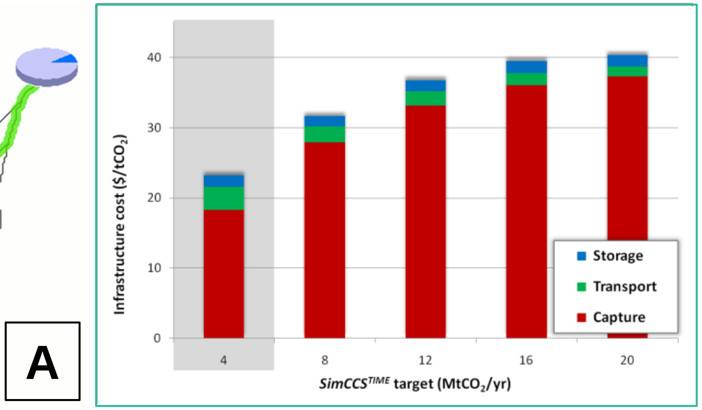


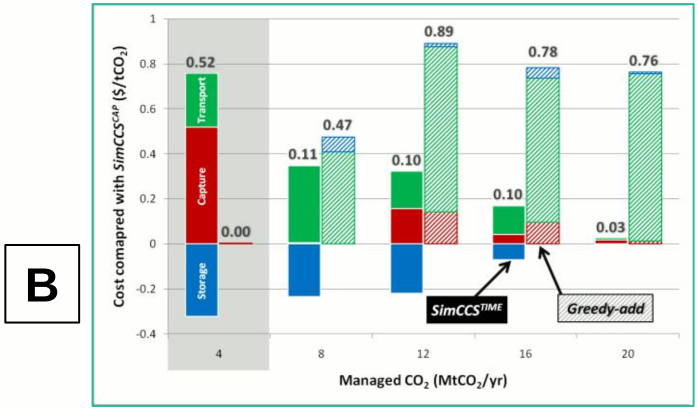
Texas panhandle

- <u>9 CO_2 sources</u> (2 biorefineries, 2 oil refineries, 2 coal and 3 natural gas stations) producing 21 $MtCO_2$/yr
- <u>3 sequestration reservoirs</u> (depleted oil fields) with 862 $MtCO_2$ capacity



Period: 1-5 years
Target: 4 $MtCO_2$/yr
Total stored: 20 $MtCO_2$





SimCCS^{TIME}

- *spatial optimization framework for* CO_2 capture and storage (CCS) infrastructure (capturing, transporting, injecting/storing CO_2) through *multiple time periods*
- deploys CCS *networks* to meet a CO_2 *cap* (i.e., cap-and-trade) or in response to a *price/tax* to emit CO_2
- intended to be used by *scientists*, CCS *stakeholders*, *policy makers*, and general *public*

Scenario

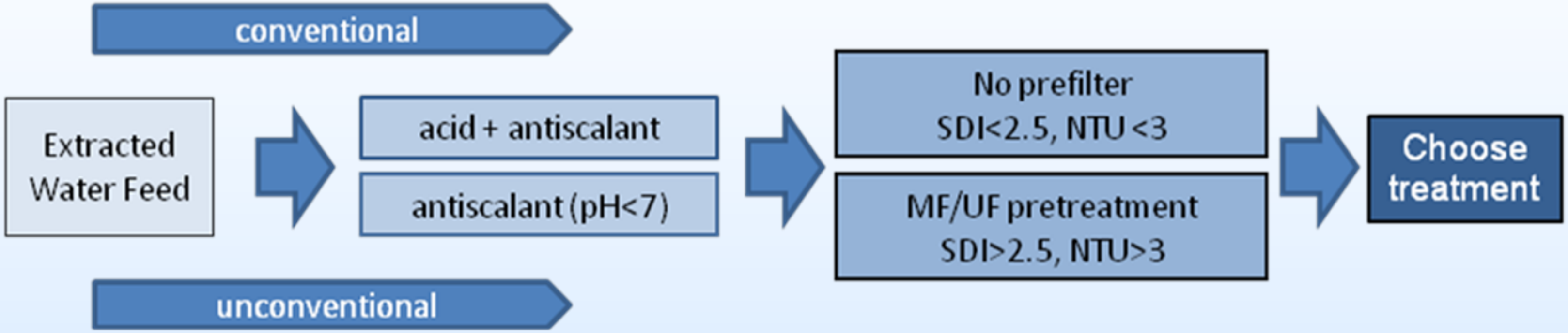
- *overbuilds infrastructure* (e.g., pipelines, capture) in early periods to achieves *long-term economies of scale*
- overall *CCS costs rise through time* as more expensive CO_2 sources are brought online, *transport costs fall* through increased utilization (<u>Chart A</u>)
- *SimCCS^{TIME}* balances CCS costs across *all time periods* while *minimizing costs* in any one time period (<u>Chart B</u>)

Water production and treatment for beneficial reuse

- Objectives
  - Minimize risks associated with pressure increase by pressure management through water production
  - Develop system modeling capabilities for assessing effective technologies and costs related to extraction and treatment of water for beneficial use
- Approach
  - Develop system modules for doing assessment while taking into account complexities
  - Apply model using real-world data from literature and from accepted water treatment practices worldwide
  - Integrate with CO_2-PENS model
- Challenges
  - Water types and sources are very different and more complex chemically than typical waters treated for municipal and industrial use
  - Obtaining complete cost data is difficult. International sources of data are very important.
  - Accounting for all costs and ancillary benefits is very specific to the capture/storage technology realm and is related to, but not the same as, typical treatment and use scenarios

Model Structure, Pretreatment and Treatment Choices

Pretreatment train


conventional

Extracted Water Feed

acid + antiscalant

antiscalant (pH<7)

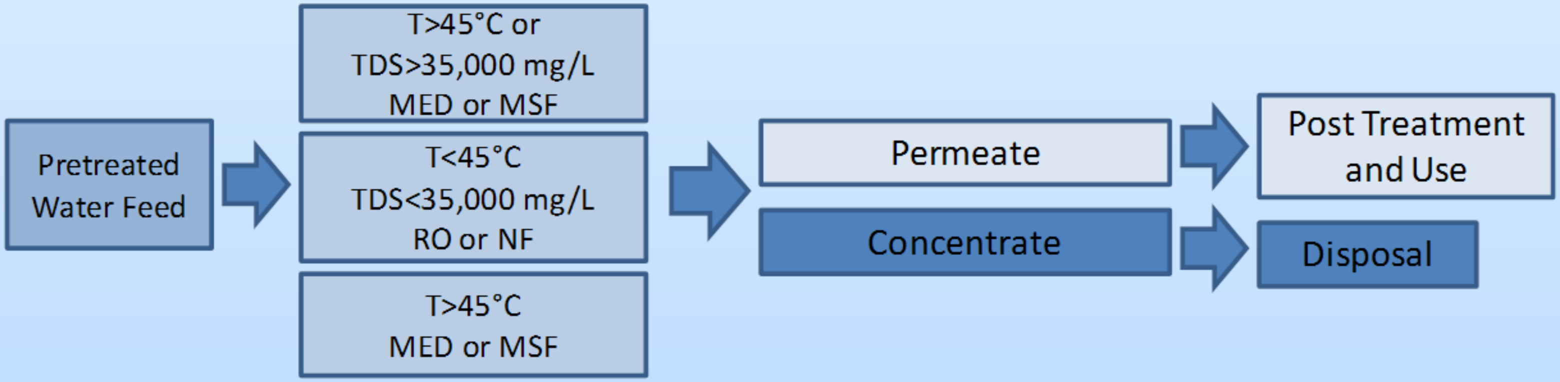
No prefilter
SDI<2.5, NTU <3

MF/UF pretreatment
SDI>2.5, NTU>3

Choose treatment

unconventional

Treatment train


Pretreated Water Feed

T>45°C or
TDS>35,000 mg/L
MED or MSF

T<45°C
TDS<35,000 mg/L
RO or NF

T>45°C
MED or MSF

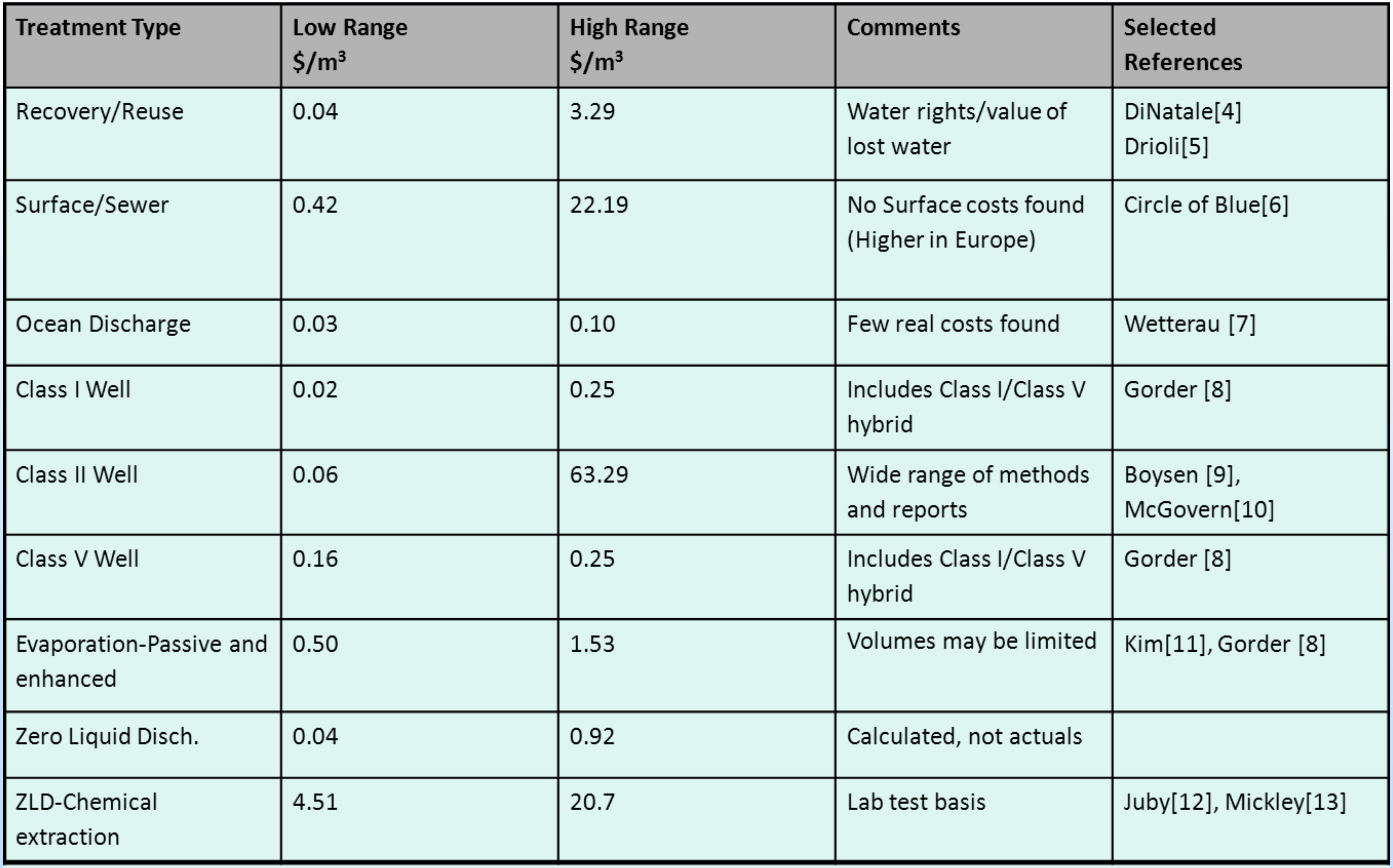
Permeate

Concentrate

Post Treatment and Use

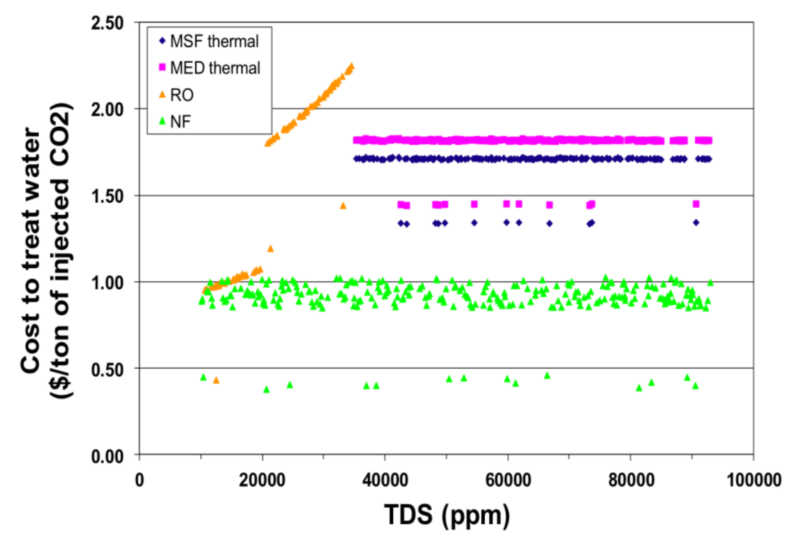
Disposal

Concentrate Disposal Options and Costs

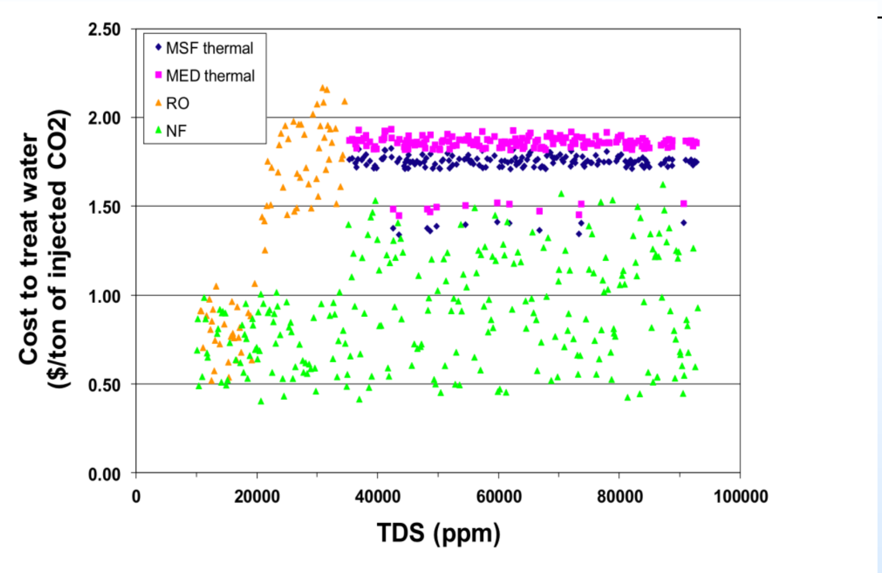


Treatment Type	Low Range $\$/m^3$	High Range $\$/m^3$	Comments	Selected References
Recovery/Reuse	0.04	3.29	Water rights/value of lost water	DiNatale[4] Drioli[5]
Surface/Sewer	0.42	22.19	No Surface costs found (Higher in Europe)	Circle of Blue[6]
Ocean Discharge	0.03	0.10	Few real costs found	Wetterau [7]
Class I Well	0.02	0.25	Includes Class I/Class V hybrid	Gorder [8]
Class II Well	0.06	63.29	Wide range of methods and reports	Boysen [9], McGovern[10]
Class V Well	0.16	0.25	Includes Class I/Class V hybrid	Gorder [8]
Evaporation-Passive and enhanced	0.50	1.53	Volumes may be limited	Kim[11], Gorder [8]
Zero Liquid Disch.	0.04	0.92	Calculated, not actuals	
ZLD-Chemical extraction	4.51	20.7	Lab test basis	Juby[12], Mickley[13]

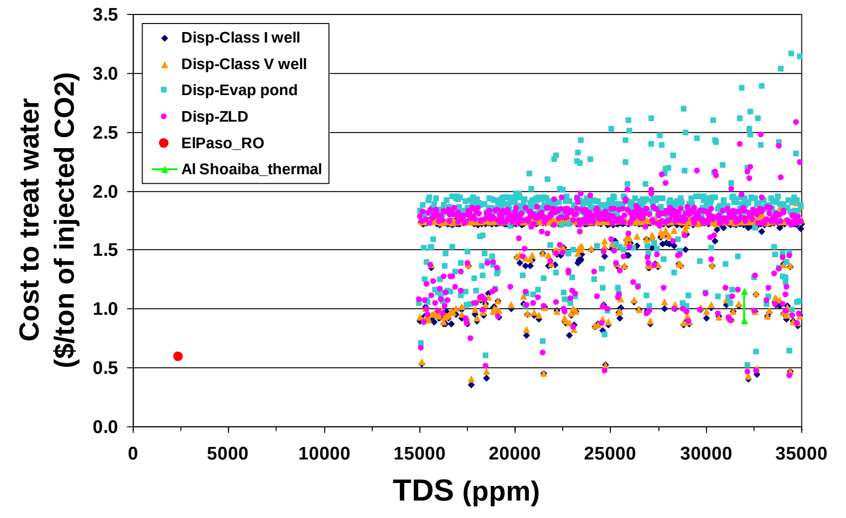
Pretreatment and concentrate disposal effects on costs



1. No pretreatment or disposal



2. Pretreatment costs added



3. Disposal costs added

As modeled, pretreatment scatters RO (±25%) and NF (±50%) ranges more than for thermal methods (±5%), probably because of the assumption that more pretreatment is used for membrane processes.

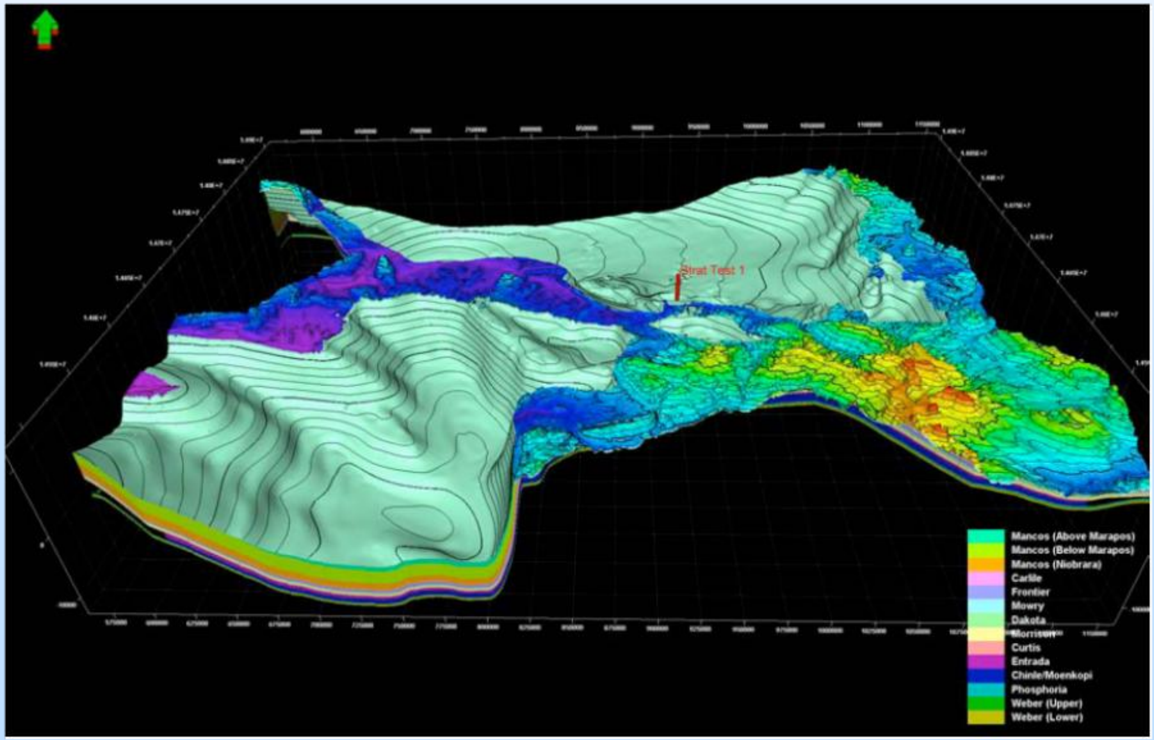
Disposal costs also scatter data and increase costs, considerably for some methods such as Class V wells.

CO_2-PENS site application

- Objectives
  - Demonstrate application of CO_2-PENS to field sites for site feasibility and long-term risks
- Approach
  - Apply CO_2-PENS to specific sites that are currently under various studies (characterization or field demonstration)
  - Update CO_2-PENS capabilities to account for site-specific issues while taking into account complexities
  - Site feasibility includes assessment of long term storage capacity, injectivity and risks
- Ongoing application
  - Craig site project led by University of Utah

Rocky Mountain Site Characterization Project: Craig site

- The project aims at regional characterization of multiple potential CO_2 sequestration target formations in Rocky Mountain region
    - Three prominent zones including Dakota sandstone, Entrada sandstone and Weber



CO_2-PENS application

- Approach:
  - Develop CO_2-PENS model for the Craig site (site-specific) and Colorado Plateau (regional)
    - Incorporate regional geologic characterization information, site-specific details
    - Potential failure pathways (wells/seals): determine probability of failures based on available data
  - Model for CO_2 sequestration reservoirs: Utilize results of numerical modeling studies: changes in reservoir pressure and saturations
  - CO_2-PENS calculations will provide results related to overall risks related to various criteria: e.g. risks of leakage of CO_2/brine
- Status:
  - Received results of numerical reservoir simulations from Univ. of Utah.
  - In process of collecting additional data (shallow formations, well/fault data)
  - In process of performing calculations on a regional basis and site-specific risks

Characterization of CO_2-water multi-phase flow

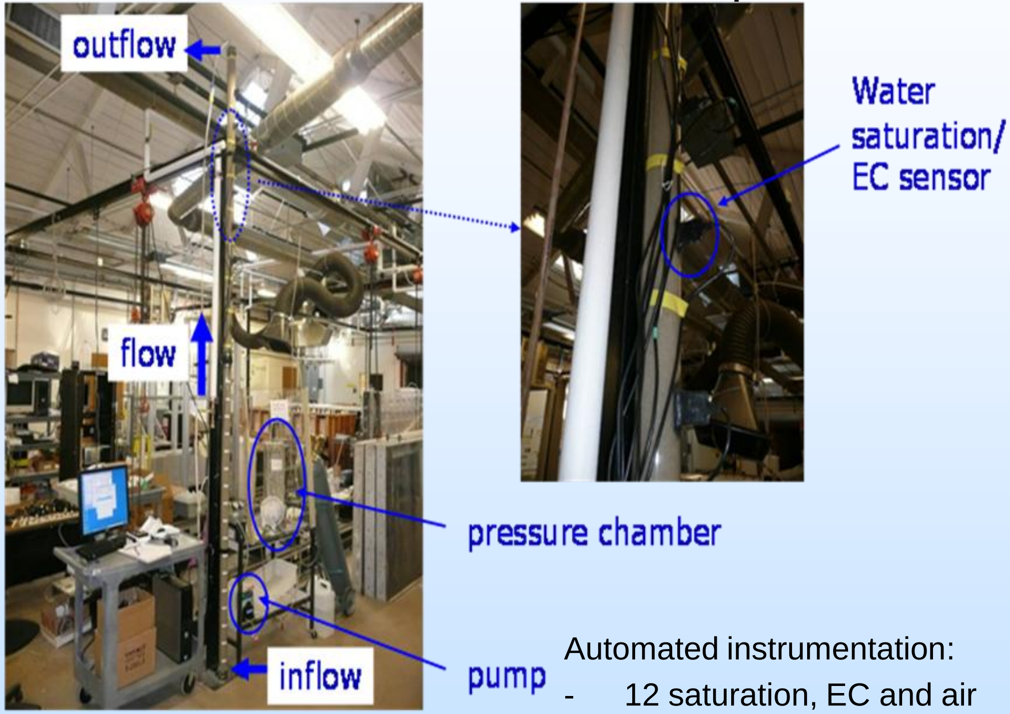
- Objectives
  - Characterize the nature of CO_2-water flow in shallow aquifer subsequent to potential leakage
  - Start filling knowledge gaps:
    - Investigate the effect of heterogeneity on the processes of CO_2 gas exsolution, expansion and migration in large systems
    - Determine how various factors affect the spatiotemporal evolution of CO_2 gas in large systems
    - Develop numerical tools for broader applications
    - Demonstrate real-world applications and upscaling effects through intermediate scale two-dimensional experiments

Characterization of CO_2-water multi-phase flow

- Approach
  - Integrated experimental and modeling approach
  - Collaboration with Prof. Tissa Illangasekare at Colorado School of Mines (CSM)
  - Unique, world-class experimental facility at CSM including sand column and two-dimensional tanks
  - Experiments under controlled conditions where CO_2-dissolved water is injected through columns/tanks under different conditions
  - Experimental results used to develop models in LANL’s FEHM simulator

Characterization of CO_2-water multi-phase flow

One dimensional sand-column experiments



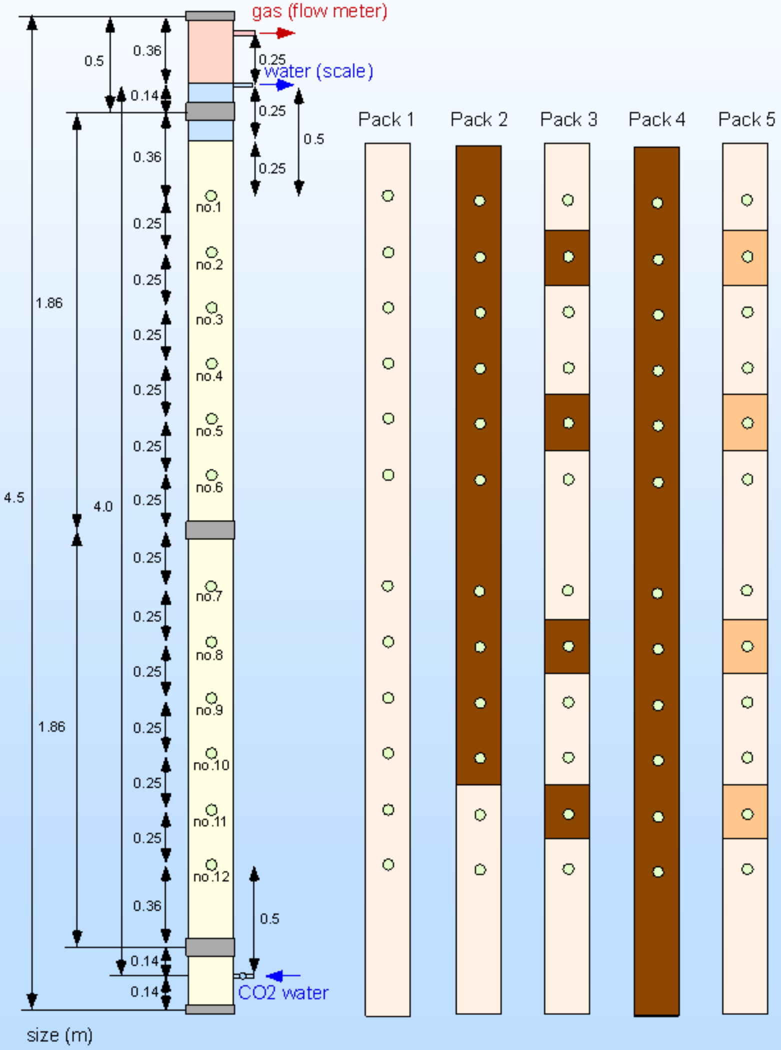
Automated instrumentation:

- 12 saturation, EC and air temperature sensors
- 14 water pressure tensiometers
- 2 soil temperature sensors
- 1 electronic balance
- 1 gas flow meter
- 1 pH meter

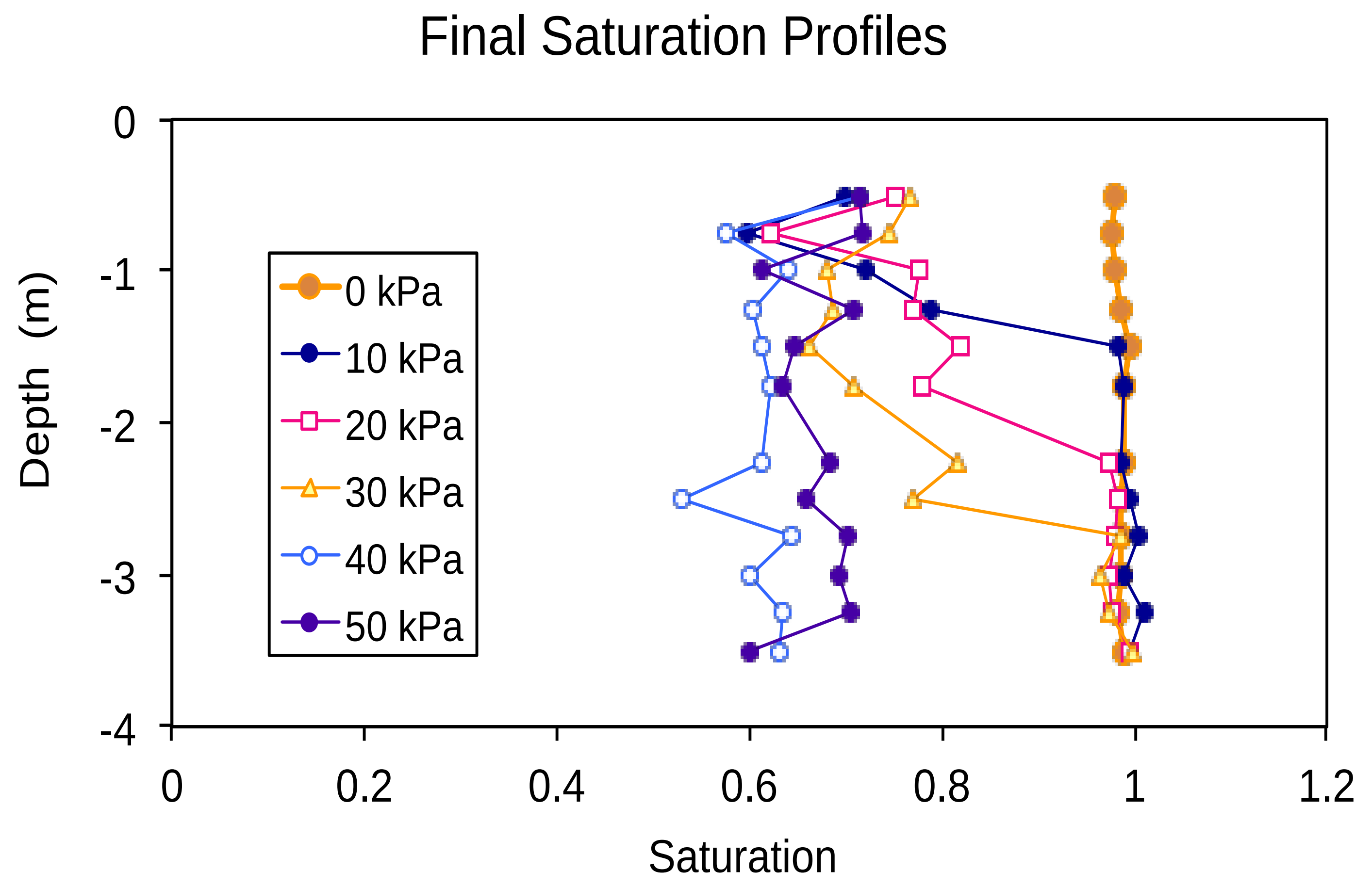
Various injected CO_2 concentrations and injection rates

Column configuration

Multiple sand-packings



Example experimental results

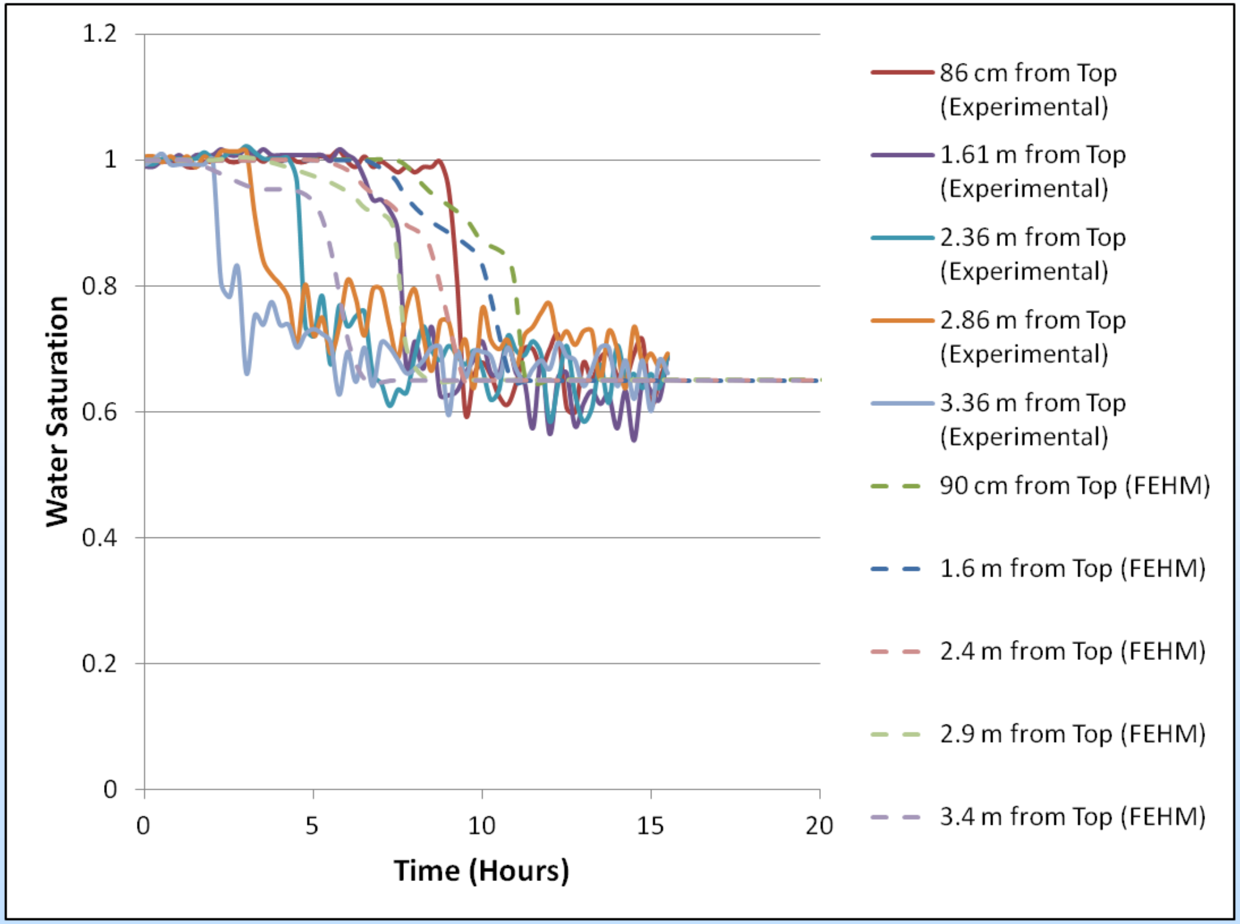


The final distribution of gas in the column depends on the saturation pressure

Results of 1-D column experiments

- The spatiotemporal pattern of CO_2 gas exsolution is relatively insensitive to injection rate
- Exsolution proceeds more slowly in fine homogeneous systems than coarse when the water is not supersaturated
- The vertical extent of the gas phase is directly proportional to the saturation pressure
- The higher the injected CO_2 concentration, the sooner and quicker the exsolution
- Heterogeneous interfaces trigger exsolution when they exist in the portion of the column where the injected water is supersaturated
- Gas accumulates under interfaces from coarse to fine sand
- Preferential flow paths occur more often through fine sand than coarse

Numerical Modeling with LANL's FEHM simulator



Injected water saturation pressure: 50 KPa

Matching experimental observations needed incorporation of 35% critical gas phase saturation

Accomplishments to Date

- CO_2-PENS, first-ever system model for CCS studies:
  - Developed capabilities for application to site-specific complex geologies
- Integrated *SimCCS* (CO_2 pipeline infrastructure optimization model) with CO_2-PENS (System model for geologic CO_2 storage): First-ever modeling approach of such kind.
- Applied integrated *SimCCS* & CO_2-PENS modeling capability to multiple sets of field data.
- Developed a comprehensive system module for assessment of water production to minimize risks and treatment for beneficial reuse.
- Completed column experiments to characterize multi-phase CO_2-water flow and developed numerical models for the experiments:
  - Experimental observations are filling-in needs.

Future Plans

- Complete developments in *SimCCS* to account for site-specific risks
- Complete application of CO_2-PENS to Craig site
- Develop capabilities in CO_2-PENS and apply to CO_2 EOR site applications
  - Oil-specific issues
- System model for water treatment:
  - Expand cost database including factors such as organic pretreatments and add benefits
  - Integration with NATCARB for water composition
  - Develop an independent tool for assessment of water production and treatment
- 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:
    - Richard Middleton: CCS Infrastructure optimization
    - Jeri Sullivan: Water treatment system modeling
    - Shaoping Chu: Water treatment system modeling
    - Hari Viswanathan: CO_2-PENS site application
    - Prof. Tissa Illangasekare (Colorado School of Mines): CO_2 release experimental characterization

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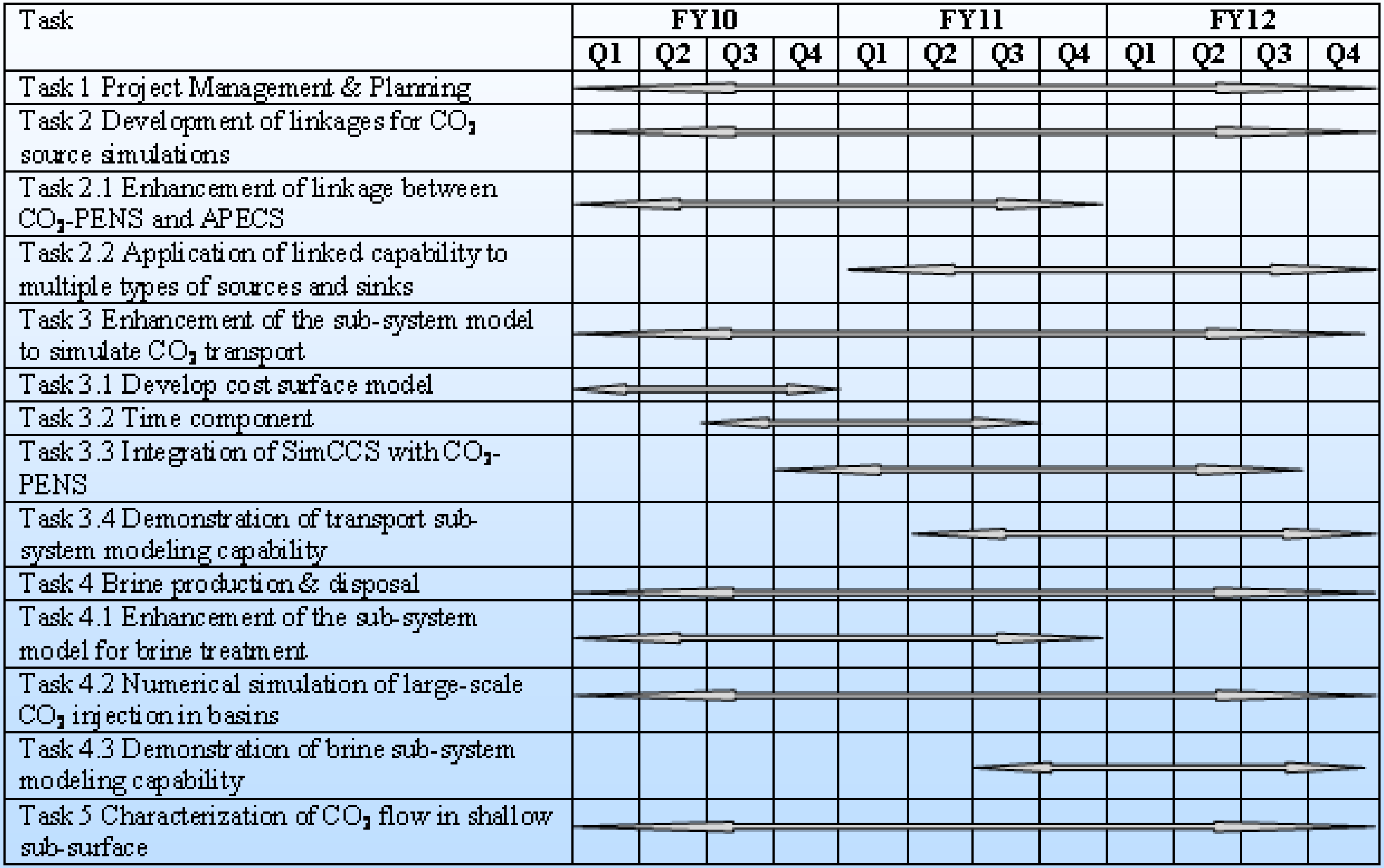
Gantt Chart



Task	FY10				FY11				FY12			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Task 1 Project Management & Planning	↔	↔	↔	↔	↔	↔	↔	↔	↔	↔	↔	↔
Task 2 Development of linkages for CO_2 source simulations	↔	↔	↔	↔	↔	↔	↔	↔	↔	↔	↔	↔
Task 2.1 Enhancement of linkage between CO_2-PENS and APECS	↔	↔	↔	↔	↔	↔	↔	↔				
Task 2.2 Application of linked capability to multiple types of sources and sinks					↔	↔	↔	↔	↔	↔	↔	↔
Task 3 Enhancement of the sub-system model to simulate CO_2 transport	↔	↔	↔	↔	↔	↔	↔	↔	↔	↔	↔	↔
Task 3.1 Develop cost surface model	↔	↔	↔	↔								
Task 3.2 Time component			↔	↔	↔	↔	↔					
Task 3.3 Integration of SimCCS with CO_2-PENS				↔	↔	↔	↔	↔	↔	↔	↔	
Task 3.4 Demonstration of transport sub-system modeling capability						↔	↔	↔	↔	↔	↔	↔
Task 4 Brine production & disposal	↔	↔	↔	↔	↔	↔	↔	↔	↔	↔	↔	↔
Task 4.1 Enhancement of the sub-system model for brine treatment	↔	↔	↔	↔	↔	↔	↔	↔				
Task 4.2 Numerical simulation of large-scale CO_2 injection in basins	↔	↔	↔	↔	↔	↔	↔	↔	↔	↔	↔	↔
Task 4.3 Demonstration of brine sub-system modeling capability							↔	↔	↔	↔	↔	↔
Task 5 Characterization of CO_2 flow in shallow sub-surface	↔	↔	↔	↔	↔	↔	↔	↔	↔	↔	↔	↔

Publications and presentations

Publications:

- 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.
- 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:

Middleton, R. S., Keating, G.N., Brandt, A.R., Viswanathan, H.S., Stauffer, P.H., Pawar, R.J., and Bielicki, J.M. (2012). CO_2 leakage risks and the impact on commercial-scale CO_2 capture, transport, and storage: Alberta oil sands case study, Eleventh Annual Conference on Carbon Capture, Utilization & Sequestration, Pittsburgh, PA.

Sullivan, E. J., Chu, S., Stauffer, P., Pawar, R. (2012). A CO_2-PENS model of methods and costs for treatment of water extracted during geologic carbon sequestration, Desalination for the Environment Clean Water and Energy, Barcelona, Spain.

Sullivan, E. J., Chu, S., Stauffer, P., Pawar, R. (2012). Thermal Treatment Costs and Cost Recovery for Water Extracted During Geologic Sequestration, Eleventh Annual Conference on Carbon Capture, Utilization & Sequestration, Pittsburgh, PA.

Middleton, R. S. and Keating, G.N. (2012). Geospatially optimizing CO_2 capture and storage infrastructure with geologic uncertainty, Annual Meeting of the Association of American Geographers, New York, NY.

Lassen, R., Sakaki, T., Plampin, M., Pawar, R., Jensen, K., Sonnenborg, T., Illangasekare, T. (2011). Study of effects of formation heterogeneity of carbon dioxide gas migration using a two-dimensional intermediate scale, Fall AGU meeting, San Francisco, CA.

Sakaki, T., Lassen R., Plampin, M., Pawar, R., Komatsu, M., Jensen, K., Illangasekare, T. (2011). A fundamental study of gas formation and migration during leakage of stored carbon dioxide in subsurface formations, Fall AGU meeting, San Francisco, CA.

Pawar, R., Dash, Z., Sakaki, T., Plampin, M., Lassen, R., Jensen, K., Illangasekare, T., Zyvoloski, G. (2011) Numerical modeling of experimental observations on gas formation and multi-phase flow of carbon dioxide in subsurface formations, Fall AGU meeting, San Francisco, CA.

Sullivan, E. J., Chu, S., Pawar, R. (2011).,Effects of Concentrate Disposal and Energy Recovery on Costs for Treatment of Water Produced During Geologic Sequestration , Tenth Annual Conference on Carbon Capture & Sequestration, Pittsburgh PA.

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Publications and presentations (continued)

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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.