Systems Modeling & Science for Geologic Sequestration
Project Number: LANL FE10-003 Task 3

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Strategic Center for Coal’s
FY10 Carbon Sequestration Peer Review
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Collaborators

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• Jacob Bauman (LANL)
• 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 CO₂ 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 CO₂ leakage in shallow aquifers. This technology contributes to the Carbon Storage Program’s effort of ensuring 99 percent CO₂ 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 CO₂ 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 CO₂-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 m³/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

Treatment train

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

- Extraction Source
- Treatment Location
- Concentrate Disposal Point
- Treated Water Point of Use

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

Water Treatment Model

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

Ocean choice
1: near ocean
2: not near ocean

Produced water choice
check: yes
unchck: no

Thermal method
1: MSF
2: ME-TVC

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

Transport mode choice
1: truck
2: pipeline
3: other

Tank flag
0: no tank
1: use tank

Pond flag
0: no pond
1: use pond

Stochastic input variable range

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
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 [$/m³] 8.04e-008
Acid rate max [$/m³] 0.0053
Antiscalent rate min [$/m³] 6.31e-009
Antiscalent rate max [$/m³] 0.0053

Cost of energy scenario

Scenario 4 cents/kWh
Scenario 10 cents/kWh
Scenario 20 cents/kWh

Permeate volume (%)

50

Incoming water amount (kg)

6700000

Org pretreat choice
1: yes

Results
## Water Module Output Dashboard

### Results

<table>
<thead>
<tr>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean final cost before disposal treatment ($)</td>
<td>21017.1 $</td>
</tr>
<tr>
<td>Mean final treated volume (m³)</td>
<td>6098.16 m³</td>
</tr>
<tr>
<td>Mean final rejected volume (m³)</td>
<td>677.573 m³</td>
</tr>
<tr>
<td>Mean final rejected water quality (ppm)</td>
<td>95501 ppm</td>
</tr>
<tr>
<td>Primary treatment method</td>
<td></td>
</tr>
<tr>
<td>Trans cost ($)</td>
<td>2532.12 $</td>
</tr>
<tr>
<td>Storage cost ($)</td>
<td>18721.4 $</td>
</tr>
<tr>
<td>Final cost + TS cost (no disposal cost included) ($)</td>
<td>37132.4 $</td>
</tr>
<tr>
<td>x1 (km)</td>
<td></td>
</tr>
<tr>
<td>x2 (km)</td>
<td></td>
</tr>
<tr>
<td>x3 (km)</td>
<td></td>
</tr>
<tr>
<td>Cost include disposal treatment (9 methods)</td>
<td></td>
</tr>
<tr>
<td>Reuse</td>
<td></td>
</tr>
<tr>
<td>Surface water discharge</td>
<td></td>
</tr>
<tr>
<td>Sewer plant</td>
<td></td>
</tr>
<tr>
<td>Ocean</td>
<td></td>
</tr>
<tr>
<td>Well class I</td>
<td></td>
</tr>
<tr>
<td>Well class II</td>
<td>56185 $</td>
</tr>
<tr>
<td>Well class V</td>
<td></td>
</tr>
<tr>
<td>Evaporation pond</td>
<td>16420.8 $</td>
</tr>
<tr>
<td>Zero liquid discharge</td>
<td>16410.4 $</td>
</tr>
</tbody>
</table>

### Calculated cost to treat water

- **Reuse**: Calculated cost to treat water ($) - reuse
- **Surface discharge**: Calculated cost to treat water ($) - surface discharge
- **Sewer plant**: Calculated cost to treat water ($) - sewer plant
- **Ocean**: Calculated cost to treat water ($) - ocean
- **Well class I**: Calculated cost to treat water ($) - well class I
- **Well class II**: Calculated cost to treat water ($) - well class II
- **Well class V**: Calculated cost to treat water ($) - well class V
- **Evaporation pond**: Calculated cost to treat water ($) - evaporation pond
- **Zero liquid discharge**: Calculated cost to treat water ($) - ZLD
Example Application to Teapot Dome

Base case: Teapot Dome\(^1\)

Q=6700 m\(^3/d\)

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).
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

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Minimum</th>
<th>Maximum</th>
</tr>
</thead>
<tbody>
<tr>
<td>Porosity</td>
<td>0.05</td>
<td>0.3</td>
</tr>
<tr>
<td>Average Permeability (md)</td>
<td>1</td>
<td>10</td>
</tr>
<tr>
<td>Thickness (ft)</td>
<td>50</td>
<td>800</td>
</tr>
<tr>
<td>Time (years)</td>
<td>5</td>
<td>50</td>
</tr>
<tr>
<td>Pmax (psi)</td>
<td>800</td>
<td>6400</td>
</tr>
<tr>
<td>Temperature (degrees F)</td>
<td>80</td>
<td>250</td>
</tr>
<tr>
<td>Mole Fractions for C1, C3-C5, C6, C10, C21, C36</td>
<td>0</td>
<td>1</td>
</tr>
</tbody>
</table>
Simulation Results

Histogram of % Oil Recovery

Histogram of Amount of CO₂ 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 CO₂ 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

% Oil Recovery

Amount of CO2 Stored

CO2 Stored (tons)
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

$\Delta P_{inj}$: Difference in the saturation pressure and hydrostatic pressure, $\Delta P_{e}$: Difference in the gas entry pressure for two sands at the heterogeneity interface

<table>
<thead>
<tr>
<th>$\Delta P_{os}$</th>
<th>Gas phase should evolve at the bottom of column, irrespective of heterogeneity</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\leq 0$</td>
<td></td>
</tr>
<tr>
<td>$&lt; \Delta P_{os,min}$</td>
<td>Gas phase will not evolve near the heterogeneity interface, the presence of heterogeneity does not have an effect on gas phase evolution</td>
</tr>
<tr>
<td>$\Delta P_{os,min} = 2P_{e, top sand} - P_{e, bottom sand} - \rho g \Delta h$</td>
<td></td>
</tr>
</tbody>
</table>
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 $\Delta P_{os} > 0$ kPa, and *after* one pore volume had been injected when $\Delta P_{os} < 0$ 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 development
    • Prof. Tissa Illangasekare (Colorado School of Mines): CO₂ release experimental characterization
    • Michael Plampin (Colorado School of Mines): CO₂ release experimental characterization
    • Mike Porter: Numerical simulation of CO₂ release experiments
Publications:

- Plampin, M., Sakaki, T., Illangasekare, T., and Pawar, R., An Intermediate-Scale Experimental Investigation into the Effects of Heterogeneity on CO₂ Gas Phase Evolution in Shallow Subsurface Environments During Leakage from Geologic Sequestration Sites, In review *International Journal of Greenhouse Gas Control*
Publications and presentations

Publications:


Presentations:


Publications and presentations (continued)

Presentations:
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 CO₂ capture and storage, perform outreach education on these issues, and to disseminate water research performed within the Capture program and the Partnerships