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

Rajesh Pawar
Los Alamos National Laboratory

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Transforming Technology through Integration and Collaboration
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Contributors

- Tissa Illangasekare (Colorado School of Mines)
- Michael Plampin (Colorado School of Mines)
- Jeri Sullivan (LANL)
- Shaoping Chu (LANL)
- Mark Porter (LANL)
- Elizabeth Keating (LANL)
- Zhenxue Dai (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:
  – Develop and validate technologies to ensure 99 percent storage permanence.
  – Develop technologies to improve reservoir storage efficiency while ensuring containment effectiveness.

• Project benefit:
  – The project is also developing science basis that can be used to assess impacts of CO\textsubscript{2} leakage in shallow aquifers and to characterize leakage through faults. This technology contributes to the Carbon Storage Program’s effort of ensuring 99 percent CO\textsubscript{2} storage permanence in the injection zone(s).
Project Overview:
Tasks

1. Characterize multi-phase CO$_2$ flow in groundwater aquifers through an integrated experimental-simulation approach
2. Characterize multi-phase CO$_2$-brine flow through faults
3. 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: Completed
   • Develop system modeling capabilities for assessment of feasibility of long-term CO$_2$ storage at CO$_2$-EOR sites: Not discussed here
Characterization of CO$_2$-water multi-phase flow
Goals & Objectives

- Understand the process of gas exsolution, gas phase expansion and CO$_2$ migration to characterize the impacts of CO$_2$ & CO$_2$-dissolved water leakage in groundwater aquifer as well as to deploy efficient monitoring/mitigation approaches
  - What factors affect the spatiotemporal evolution of CO$_2$ migration
  - What role does heterogeneity play
  - Data to develop theory
- Integrated approach: intermediate scale experiments (1D column, 2D tank) coupled with numerical simulations
- Measurements taken from sensors, flow meters and scales every minute
- Aqueous phase samples taken at various intervals and analyzed for dissolved CO$_2$ with an Ion Chromatograph
Experimental Setup

~ 2.5 months to pack and configure the tank
Experimental Conditions

- CO$_2$-dissolved water injected for 2 days
- Continued observations for >30 days
Observed Dissolved CO$_2$ Migration

only the “lower aquifer” (region below fine sand layer) is shown
Observed Gaseous CO₂ Evolution

only the “lower aquifer” (region below fine sand layer) is shown
Macroscopic CO$_2$ Mass Balance

~13.6 % of injected CO$_2$ remained inside the tank

Negligible release of gas phase CO$_2$ to the atmosphere (gas phase was "trapped" under the fine layer)
Key Findings

• Permeability contrast (heterogeneity) affects CO$_2$ gas phase migration:
  – Under the conditions of buoyancy-dominated flow even lower permeability sands can help prevent upward migration of gaseous CO$_2$

• Background flow affects the existence of free-phase CO$_2$:
  – Higher fraction of CO$_2$ in dissolved-form

• Dissolved CO$_2$ plume primarily remains at the bottom

• CO$_2$ remains in the water (primarily dissolved) well after leakage stops

• Important implications on monitoring and mitigation
• Flow rates were taken from linear regressions of experimental cumulative water outflow curves
Simulation Results: Dissolved CO$_2$ Migration

only the "lower aquifer" (region below fine sand layer) is shown
Simulation Results: Gaseous CO$_2$ Evolution

only the “lower aquifer” (region below fine sand layer) is shown
Numerical Model Sensitivity Analysis

- **Lower air entry pressure**
  - Gas Saturation
  - Simulation: \( t = 1.75 \) days

- **Higher residual gas saturation**
  - Gas Saturation
  - Simulation: \( t = 1.75 \) days

- **Higher saturation pressure**
  - Gas Saturation
  - Simulation: \( t = 1.75 \) days

- **All three parameters adjusted**
  - Gas Saturation
  - Simulation: \( t = 1.75 \) days

Each image shows the gas phase near the end of the \( \text{CO}_2 \)-water injection period.
Characterization of multi-phase CO$_2$-brine flow along faults
Objectives

• Activation/rupture of faults and subsequent leakage of CO$_2$ is one of the concerns related to containment (Zoback & Gorelick, 2012)

• Using numerical simulations our objective is to answer:
  ➢ Can the rupture be detected with pressure monitoring in the reservoir?
  ➢ How much CO$_2$ might leak upward through the ruptured fault before detection?
  ➢ How does the process of CO$_2$/brine flow through the complex fault geology evolve?
Approach

Numerical simulations using FEHM:
1. Reservoir-scale simulations of CO₂/brine migration along faults post-rupture due to overpressurization
   • Scenario: activation of a critically stressed “unknown” fault
   • Fault rupture process not explicitly modeled
   • Permeability of fault increased in over-pressure exceeded “critical” threshold
   • Monte-Carlo simulations varying a range of parameters

2. Fault-scale simulations of reactive transport of CO₂ in heterogeneous fault zones
   • Explicitly simulate heterogeneous damage zone, fault core
   • Determine impact of self-sealing driven by depressurization, degassing, and calcite precipitation
Conceptual Model for Fault Rupture Simulations

Monte-Carlo Simulations

<table>
<thead>
<tr>
<th>Variable</th>
<th>Min</th>
<th>Max</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Distance from injector to fault</td>
<td>1000</td>
<td>5000</td>
<td>m</td>
</tr>
<tr>
<td>Fault width</td>
<td>1</td>
<td>50</td>
<td>m</td>
</tr>
<tr>
<td>Reservoir permeability</td>
<td>-15</td>
<td>-12</td>
<td>Log (m²)</td>
</tr>
<tr>
<td>Overpressure at injection well</td>
<td>2</td>
<td>15</td>
<td>MPa</td>
</tr>
<tr>
<td>Critical overpressure for fault rupture</td>
<td>0.5</td>
<td>10</td>
<td>MPa</td>
</tr>
</tbody>
</table>

Wide range of scenarios: ~ 200 Simulations Runs
Example Simulation Result

~ 3 years after rupture.

Free-phase CO$_2$ plume migration

Dissolved CO$_2$ plume migration
Key Findings

- In the large majority of cases, fault rupture is readily detectible by rapid pressure drop at the injection well.
  - In 98% cases pressure at injection well decreased by $> 300$ KPa.

- There are significant delays between rupture and CO$_2$ plume breakthrough at base of fault. In most cases, free-phase CO$_2$ plume had not reached base of fault 5 years post-rupture.
Numerical studies of CO₂ and brine leakage along faults

Fault-scale simulations of reactive transport of CO₂ in heterogeneous fault zones
- Capture effect of complexity in fault geology: core, damage zone
- Coupled processes: multi-phase flow, phase change, CO₂/brine dissolution/precipitation, density change

Preliminary results:
- Heterogeneity within the fault zone affects gas phase evolution and migration
- “Self-sealing” caused by degassing and calcite precipitation is unlikely to reduce permeability/porosity significantly on relevant time scales
Accomplishments to Date

• Developed system model for produced water treatment (CO₂-PENS WTM): Available for public use
• Completed 1-D column experiments as well as related simulations and 1 set of 2-D tank experiments on post CO₂ leakage multi-phase flow in groundwater aquifer
• Developed ROM for CO₂ storage capacity estimation during EOR operations
• Completed study on applicability of pressure monitoring for fault rupture detection
• Initiated study on characterization of coupled processes during CO₂ & brine leakage along fault capturing fault geologic complexity
• 7 Peer-reviewed journal publications, 1 journal article in press, 2 journal articles under preparation (to be submitted to IJGGC)
• Multiple presentations at international meetings: 2015 InterPORE, 2014 Fall AGU (2), GHGT12 (4), 2014 IEAGHG Joint Network Meeting, 2014 CCSU meeting (4), 2013 Fall AGU (3).
Synergy Opportunities

• Collaboration on groundwater leakage characterization and impacts: NETL
• Collaboration on development of reduced order models for estimating storage capacity during CO$_2$-EOR operations: EERC, Battelle, Princeton, U. Wyoming
Key Findings, Future Plans

- Significant results with practical implications:
  - Groundwater leakage impacts, fault rupture monitoring
- Extensive experimental data on CO$_2$-brine leakage in 1-D columns: available for model development and testing

**Future Plans:**

- Complete 2-D tank experiments with increased complexity (heterogeneous sand packing) and associated numerical simulations:
  - Data sets and parametric analysis on effect of groundwater hydrologic parameters on CO$_2$ migration and implications on monitoring/mitigation
- Complete fault flow characterization study to include fault complexities
  - Development of relationships to calculate effective CO$_2$ leakage rates along faults incorporating fault complexities
- Complete development of reduced order models to calculate CO$_2$ storage capacity during EOR operations
Organizational Chart

- PI: Rajesh Pawar
- Program Manager: George Guthrie
- Team Members:
  - Jeri Sullivan: Water treatment system modeling
  - Shaoping Chu: Water treatment system modeling
  - 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
  - Elizabeth Keating: Fault flow characterization
  - Zhenxue Dai: ROM for CO₂ storage capacity in EOR


Bibliography


