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

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Contributors

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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:
 - The project is also developing science basis that can be used to assess impacts of CO₂ leakage in shallow aquifers and to characterize leakage through faults. This technology contributes to the Carbon Storage Program's effort of ensuring 99 percent CO₂ storage permanence in the injection zone(s).

Project Overview: Tasks

- 1. Characterize multi-phase CO₂ flow in groundwater aquifers through an integrated experimental-simulation approach
- 2. Characterize multi-phase CO₂-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 CO₂ storage at CO₂-EOR sites: Not discussed here

Characterization of CO₂-water multi-phase flow

Goals & Objectives

- Understand the process of gas exsolution, gas phase expansion and CO₂ migration to characterize the impacts of CO₂ & CO₂-dissolved water leakage in groundwater aquifer as well as to deploy efficient monitoring/mitigation approaches
 - What factors affect the spatiotemporal evolution of CO₂ migration
 - What role does heterogeneity play
 - Data to develop theory
- Integrated approach: intermediate scale experiments (1D column, 2D tank) coupled with numerical simulations

2-D Tank Experimental Setup



- Measurements taken from sensors, flow meters and scales every minute
- Aqueous phase samples taken at various intervals and analyzed for dissolved CO₂ with an Ion Chromatograph

Experimental Setup





~ 2.5 months to pack and configure the tank

Experimental Conditions



Observed Dissolved CO₂ 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 CO₂ Mass Balance



Key Findings

- Permeability contrast (heterogeneity) affects CO₂ gas phase migration:
 - Under the conditions of buoyancy-dominated flow even lower permeability sands can help prevent upward migration of gaseous CO₂
- Background flow affects the existence of free-phase CO₂:
 - Higher fraction of CO₂ in dissolved-form
- Dissolved CO₂ plume primarily remains at the bottom
- CO₂ remains in the water (primarily dissolved) well after leakage stops
- Important implications on monitoring and mitigation

Numerical Model Setup: FEHM



 Flow rates were taken from linear regressions of experimental cumulative water outlow curves

Simulation Results: Dissolved CO₂ Migration



only the "lower aquifer" (region below fine sand layer) is shown

Simulation Results: Gaseous CO₂ Evolution



only the "lower aquifer" (region below fine sand layer) is shown

Numerical Model Sensitivity Analysis



Each image shows the gas phase near the end of the CO₂-water injection period

Characterization of multi-phase CO₂-brine flow along faults



- Activation/rupture of faults and subsequent leakage of CO₂ 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 CO₂ might leak upward through the ruptured fault before detection?
 - How does the process of CO₂/brine flow through the complex fault geology evolve?



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





Details in Keating, E.H., Dai, Z., Dempsey, D. Pawar, R. 2014. Effective detection of CO_2 leakage: a comparison of groundwater sampling and pressure monitoring, Energy Procedia, 63, 4163-4171.

Monte-Carlo Simulations

Variable	Min	Мах	Unit
Distance from injector to fault	1000	5000	m
		50	
Fault width	1	50	m
Reservoir permeability	-15	-12	Log (m2)
Overpressure at injection well	2	15	MPa
Critical overpressure for fault rupture	0.5	10	MPa

Wide range of scenarios: ~ 200 Simulations Runs

Example Simulation Result

~ 3 years after rupture.

Free-phase CO₂ plume migration

Dissolved CO₂ 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 CO₂ plume breakthrough at base of fault. In most cases, freephase CO₂ 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 CO_2 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 CO₂-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 CO₂-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 CO₂ migration and implications on monitoring/mitigation
- Complete fault flow characterization study to include fault complexities
 - Development of relationships to calculate effective CO₂ leakage rates along faults incorporating fault complexities
- Complete development of reduced order models to calculate CO₂ storage capacity during EOR operations

Appendix

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

- Plampin, M., Lassen, R., Sakaki, T., Porter, M., Pawar, R., Jensen, K., and Illangasekare, T., Heterogeneity-Enhanced Gas Phase Formation in Shallow Aquifers During Leakage of CO₂-Saturated Water from Geologic Sequestration Sites, Water Resources Research, 50, 9251-9266, 2015.
- Sullivan, E.J., Chu, S., Pawar, R., Probabilistic cost estimation methods for treatment of water extracted during CO₂ storage and EOR, accepted for publication by International Journal of Greenhouse Gas Control.
- Porter, M., Pawar, R., Plampin, M., Illangasekare, T., CO₂ leakage in • shallow aquifers: A benchmark modeling study of CO₂ gas evolution in heterogeneous porous media, International Journal of Greenhouse Gas Control, 39, 51-61, 2015.
- Plampin, M., Illangasekhare, T., Sakaki, T., Pawar, R., Experimental study of gas evolution in heterogeneous shallow subsurface formations during leakage of stored CO₂, International Journal of Greenhouse Gas Control, 22, 47-62, 2014. 32

Bibliography

- Keating, E.H., Dai, Z., Dempsey, D. Pawar, R., Effective detection of CO₂ leakage: a comparison of groundwater sampling and pressure monitoring, Energy Procedia, 2014, 63, 4163-4171.
- Porter, M., Plampin, M., Pawar, R., Illangasekare, T., CO₂ leakage into shallow aquifers: Modeling CO₂ gas evolution and accumulation at interfaces of heterogeneity, Energy Procedia, 2014, Vol. 63, pp. 3253-3260.
- Sullivan, E. J., Chu, S. P., Pawar R. J., Stauffer, P. H., The CO₂-PENS water treatment model: evaluation of cost profiles and importance scenarios for brackish water extracted during carbon storage, Energy Procedia, 2014, Vol. 63, pp. 7205-7214.
- Plampin, M., Porter, M., Pawar, R., Illangasekare, T., Multi-scale experimentation and numerical modeling for process understanding of CO₂ attenuation in the shallow subsurface, Energy Procedia, 2014, Vol. 63, pp. 4824-4833.

Bibliography

- Sakaki, T., Plampin, M. R., Pawar, R., Komatsu, M., Illangasekare, T. H., What controls carbon dioxide gas phase evolution in the subsurface? ~ Experimental observations in a 4.5m-long column under different heterogeneity conditions, International Journal of Greenhouse Gas Control, pp. 66-77, doi:10.1016/j.ijggc.2013.03.025, 2013.
- Sullivan, E. J., Chu, S., Stauffer, P., Middleton, R., Pawar, R., A method and cost model for treatment of water extracted during geologic CO₂ sequestration, International Journal of Greenhouse Gas Control, 12, 372-381, 2013.
- Sullivan, E. J., Chu, S., Pawar, R., Stauffer, P., A CO₂-PENS model of methods and costs for treatment of water extracted during geologic carbon sequestration, Desalination and Water Treatment, DOI:10.1080/19443994.2012.714727.