Simulation of Coupled Processes of Flow, Transport, and Storage of CO_2 in Saline Aquifers

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Developing the Technologies and Building the Infrastructure for CO_2 Storage
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Presentation Outline

- Benefit to the Program
- Project Overview: Goals and Objectives
- Technical Status
- Accomplishments to Date
- Summary
- Appendix

Benefit to the Program

- Advanced simulation tool for quantifying transport in geological formations during CO_2 sequestration that includes all mechanisms: convection, diffusion/dispersion, dissolution, and chemical reactions
- A simulator that can fully model these processes does not currently exist
- Simulator will contribute to our ability to predict CO_2 storage capacity in geologic formations, to within ±30 percent

Project Overview:
Goals and Objectives

Comprehensive reservoir simulator for investigation of CO_2 non-isothermal, multiphase flow and long-term storage in saline aquifers

1) Three-phase non-isothermal module for CO_2-brine flow
2) Coupling fluid flow and pressure with rock deformation
3) Geochemical reactions between injected CO_2 and aquifer rock
4) Modeling of density instability at CO_2-brine interface
5) Development of efficient parallel computing algorithms
6) Development of general fracture conceptual models
7) Verification and application using lab and field data

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Technical Status

1) Three-phase non-isothermal module for CO_2-brine flow

- Developed TOUGH2 fluid property module for brine-CO_2 systems
- Called ECO2M, uses fluid property correlations from earlier ECO2N module, and distinguishes between gaseous and liquid CO_2 phases
- Wrote documentation (user's manual) for module, including test problems
- Transferred code for testing

ECO2M Phase Combinations

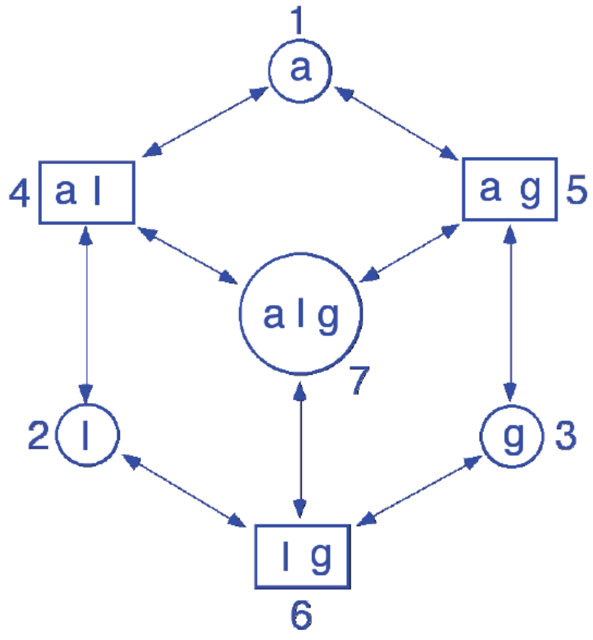


Figure 1. Possible fluid phase combinations in the system water-CO_2, and transitions between them in the P-T range of ECO2M. The phase designations are a - aqueous, l - liquid CO_2, g - gaseous CO_2. Separate liquid and gas phases of CO_2 exist only at subcritical conditions. Phase combinations are identified by a numerical index that ranges from 1 to 7.

2) Coupling fluid flow and pressure with rock deformation

- Literature review – obtain correlations describing how rock properties change with effective stress, P, and T
- Derived mean stress equation for elastic porous media
- Incorporated above into existing fluid and heat flow simulator (starting point is TOUGH2-MP)
- Simulator validation using analytical solutions (Mandel-Cryer, one-dimensional consolidation) and problems from the literature (CO_2 injection and surface uplift in the water leg of a depleting gas field; simulation of deformation and fluid circulation in a volcanic caldera structure)

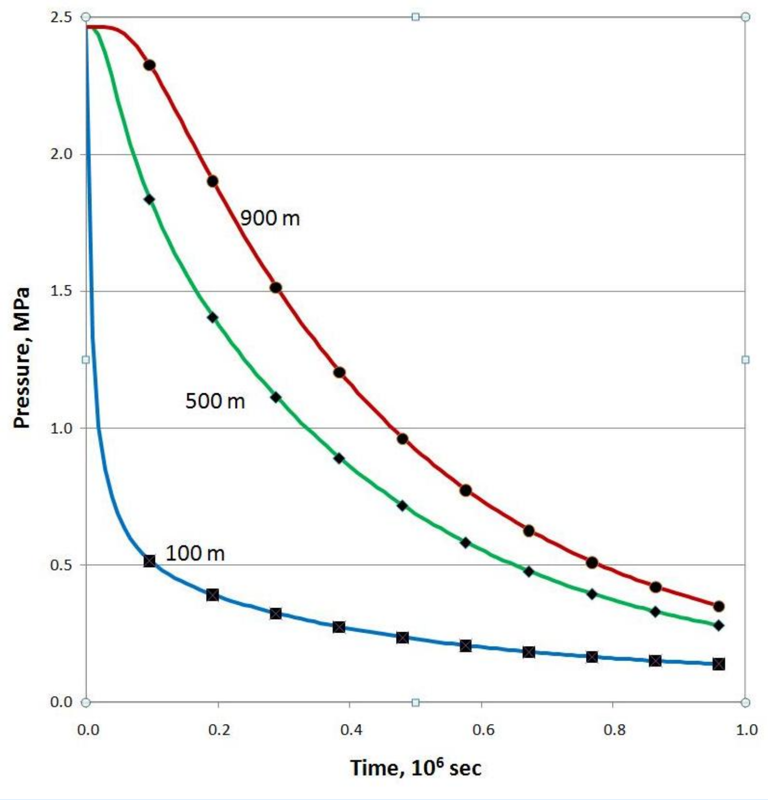
Mean Stress Equation

- = Hooke's law for a thermoporoelastic medium +
  Equations of stress equilibrium +
  Strain tensor definition
- Mean stress equation solved fully implicitly along with mass and energy balances

$$\frac{3(1-\nu)}{(1+\nu)}\nabla^2\tau_m = -\nabla\cdot\bar{F} + \frac{2(1-2\nu)}{(1+\nu)}(\alpha\nabla^2 p + 3\beta K\nabla^2 T)$$

One-Dimensional Consolidation

- Fluid-filled porous column
- Apply load to top, causing pressure to rise
- Fluid then drains out of top and pressure increase dissipates
- Simulation and analytical solution compared

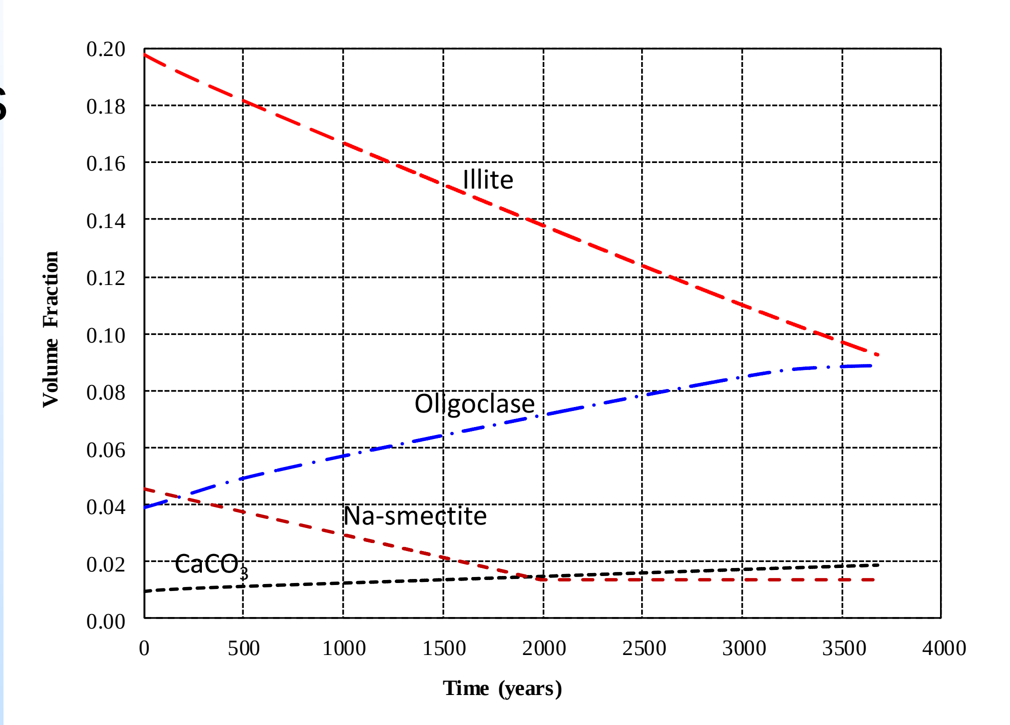


3) Geochemical reactions between injected CO_2 and aquifer rock

- Literature survey: formation brine and aquifer rock chemical composition in CO_2 sequestration projects, geochemical reaction modeling of CO_2 sequestration
- Selected fully coupled approach for reactive solute transport model; TOUGHREACT as starting point
- Fully coupled approach: solve fluid flow, solute transport, and geochemical reactions simultaneously
- A batch reaction model is simulated and compared to TOUGHREACT simulator

Batch Reaction Model

- Mineral composition typically found in sedimentary basins
- 14 kinetic chemical reactions
- 12 primary chemical species (H_2O, H^+, Ca^{2+}, Na^+, HCO_3^-, Cl^-, Mg^{2+}, K^+, Fe^{2+}, $SiO_2(aq)$, SO_4^{2-},AlO^{2-})
- 30 aqueous equilibrium reactions and secondary aqueous chemical species
- Good agreement with TOUGHREACT



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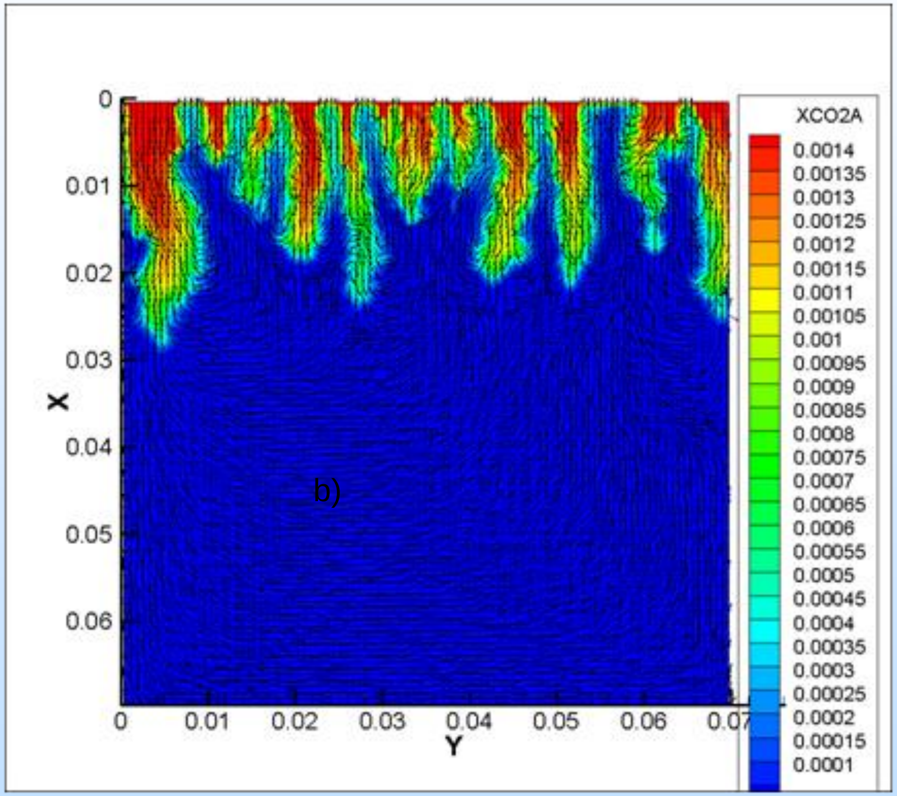
4) Modeling of density instability at CO_2-brine interface

- Literature review: density driven convective flow, instability of systems with CO_2 dissolution, diffusion, and convection
- Convective mixing simulations based on laboratory experiments:
    a) supercritical CO_2 circulated above brine-saturated packed sand in a pressure vessel
    b) CO_2 dissolves into the upper part of the saturated sand
    c) liquid phase density increases there, causing instability and setting off convective mixing
- Simulation of two-dimensional flow between parallel plates, permeability assigned randomly
- Calibrate the model to match simulation and experiment

Instability Simulation

- Hele-Shaw cell (slit flow)
- 100 × 100 grid, random permeability distribution
- Top initialized with CO_2
- Rest initialized with water
- At 500 hours the fingers are well established

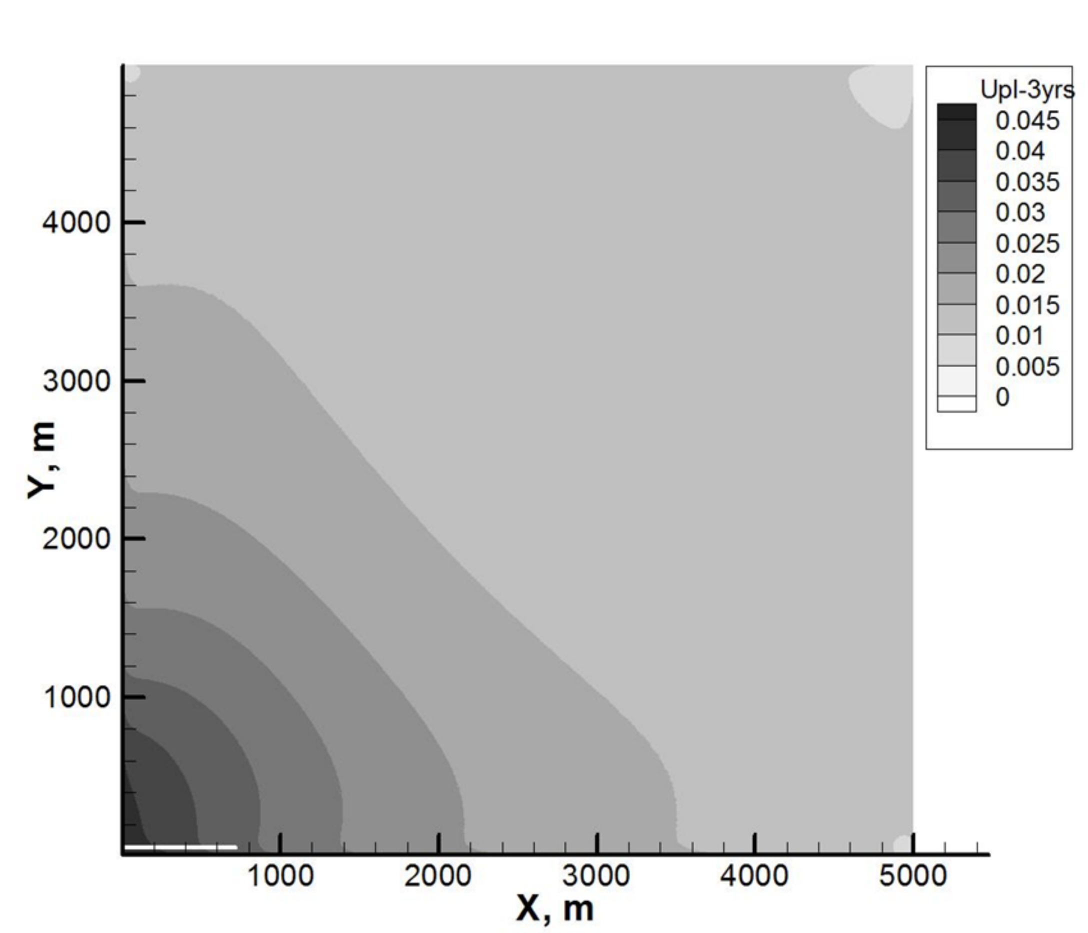


5) Development of efficient parallel computing algorithms

- Studied code parallelization including grid block partitioning, Jacobian matrix assembly, and matrix solution
- Named modified TOUGH2-MP simulator (fluid and heat flow with rock deformation) TOUGH2-CSM
- Modified TOUGH2-CSM to allow it to handle larger simulations (O[10^7-10^8] grid blocks) efficiently
- Purchased cluster computer (16 nodes, 16 processors/node (Intel ® 5260 2.4 GHz), 24 GB memory/node) to run TOUGH2-CSM on

In Salah Gas Project

- Located in Algeria
- CO_2 injected into the water leg of a depleted gas field for storage
- Simulations based on Rutqvist et al. (2010)
- Simulated surface uplift; 1000 x 1000 x 60 grid; horizontal well @ origin; (1/4) symmetry element



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6) Development of general fracture conceptual models

- Literature survey on various fractured reservoir modeling methodologies (explicit implementation of discrete fractures, multiple interacting continuum (MINC))
- Derived mean stress equation for MINC media
- Variables associated with control volume: pressure, mass fractions, and temperature for each MINC block; mean stress common to all MINC blocks
- Incorporated MINC model into TOUGH2-CSM
- Validation using analytical solution for one-dimensional consolidation in double porosity deformable media

Idealized MINC Grid

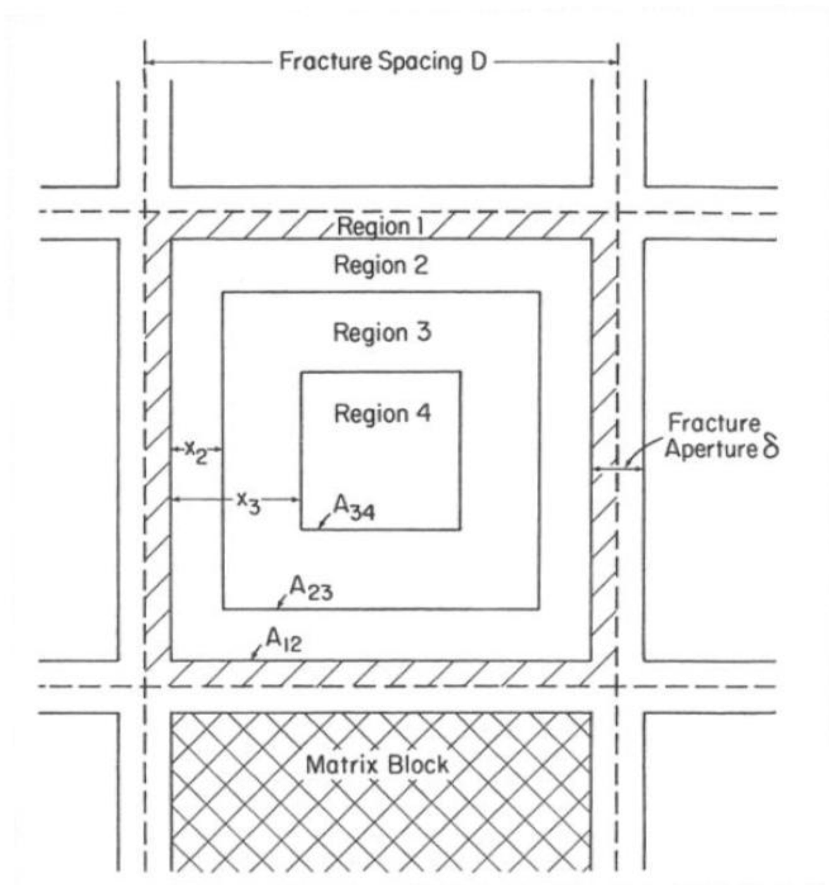

Figure 10: MINC partitioning of an idealized fracture system [Pruess, 1983]

Accomplishments to Date

- Developed ECO2M fluid property module with aqueous, and gaseous and liquid CO_2 phases
- Wrote parallel, fully coupled simulator (TOUGH2-CSM) with fluid and heat flow, and geomechanical effects in fractured and porous media, using TOUGH2-MP as the starting point
- Wrote fully coupled geochemical reaction model using TOUGHREACT as the starting point
- Studied and simulated density-driven instability

Summary

- Project is on schedule and on budget as planned
- Simulator development is mostly completed
- Future work will emphasize verification and application using lab and field data, and transferring simulation technology to users

Appendix

Organization Chart

Colorado School of Mines

Jeffery Chen, Assistant Professor of Computer Science
Philip Winterfeld, Research Associate Professor, Petroleum Eng.
Yu-Shu Wu, Prof. and CMG Reservoir Modeling Chair, Pet. Eng.
Xiaolong Yin, Assistant Professor, Petroleum Engineering
Ronglei Zhang, Ph.D. Candidate, Petroleum Engineering

Computer Modeling Group
(CMG)
Industry sponsor

Lawrence Berkeley National Laboratory

Karsten Pruess, Senior Scientist, Hydrogeology (retired)
Curt Oldenburg, Staff Geological Scientist and Head Geologic Carbon Sequestration Program, Hydrogeology

Gantt Chart

Year	Year 1				Year 2				Year 3				Year 4			
Quarter	1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4
Task 2: Three-phase CO2 module																
Task 2.1 Implement fluid property correlations																
Task 2.2 Develop phase change capabilities																
Task 2.3 Finalize coding and documentation																
Task 3: Rock deformation module																
Task 3.1 Literature review																
Task 3.2 Formulation and coding																
Task 3.2 Program and initial verification																
Task 3.3 Implementation and verification																
Task 3.4 Integration and application																
Task 4: Identification and modeling of important geochemical reactions																
Task 4.1 Survey of important reactions																
Task 4.2 Study of kinetics in a fracture																
Task 4.3 Investigation of rxn in non aq. phase																
Task 4.4 Reaction module development																
Task 5: Characterization and modeling of dissolution-driven instability																
Task 5.1 Survey and analysis of existing data																
Task 5.2 Theoretical and numerical studies																
Task 5.3 Modeling of instability and integration																

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Gantt Chart,Cont'd

Year	Year 1				Year 2				Year 3				Year 4			
Quarter	1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4
Task 6: Parallel computing scheme																
Task 6.1 Literature review																
Task 6.2 Grid partitioning																
Task 6.3 Grid block reordering																
Task 6.4 Jacobian matrix calculations																
Task 6.5 Parallel linear system solver																
Task 6.6 Implementation																
Task 6.7 Software test																
Task 6.8 Software release																
Task 7: Fracture models																
Task 7.1 Literature review																
Task 7.1 Conceptual model development																
Task 7.2 Formulation and coding																
Task 7.2 Programming and testing																
Task 7.3 Verification and improvement																
Task 7.4 Integration and application																
Task 8: Verification and Application																
Task 8.1 Against other simulators																
Task 8.2 Against lab data																
Task 8.3 Against field data																

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