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

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U.S. Department of Energy

National Energy Technology Laboratory
Carbon Storage R&D Project Review Meeting
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 porous and fractured geological formations during CO_2 sequestration that includes all mechanisms: convection, diffusion, 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

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

- TOUGH2 fluid property module - brine-CO_2 systems
- Called ECO2M, uses fluid property correlations from earlier ECO2N module
- Developed for CO_2 sequestration, highly accurate for conditions of interest (10 - 110 °C, P < 600 bar)
- Three phases: aqueous, liquid CO_2-rich, gaseous CO_2-rich; plus two- and three-phase combinations
- Wrote documentation (user's manual) for module, including test problems, tested code

ECO2M Phase Combinations

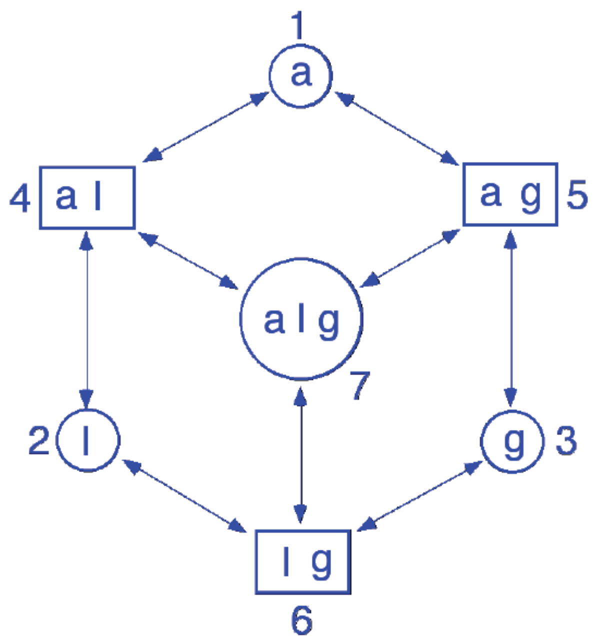

Figure 1. Possible fluid phase combinations in the system water-CO_2, and transitions between them in the P-T range of ECO2M. The phase designations are a - aqueous, l - liquid CO_2, g - gaseous CO_2. Separate liquid and gas phases of CO_2 exist only at subcritical conditions. Phase combinations are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

2) Coupling fluid flow and pressure with rock deformation

- Fully coupled simulator, TOUGH2-CSM, for modeling THM effects in fractured and porous media saline aquifers
- Based on TOUGH2-MP formulation, geomechanical effects modeled using Mean Stress Equation
- Porosity and permeability depend on effective stress
- Validated using analytical solutions (Mandel-Cryer, one-dimensional consolidation) and studies from the literature

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Geomechanical Formulation

- Combine Hooke's law for a thermo-multi-poroelastic medium, stress equilibrium equation and strain tensor definition to yield Mean Stress Equation

$$\frac{3(1-\nu)}{1+\nu}\nabla^2\tau_m + \nabla\cdot\bar{F} - \frac{2(1-2\nu)}{1+\nu}\nabla^2\left[\sum_k (\alpha_k P_k + 3\beta K \omega_k T_k)\right] = 0$$

- Trace of Hooke's law: volumetric strain equation

$$K\epsilon_v = \tau_m - \sum_k \left(\alpha_k P_k + 3\beta K \omega_k (T_k - T_{ref})\right)$$

Rock Property Correlations

- Φ and k correlate with effective stress: $\tau' = \tau_m - \alpha P$
- Rutqvist et al. (2002)

$$\phi = \phi_r + (\phi_0 - \phi_r)e^{-a\tau'} \qquad k = k_0 e^{c\left(\frac{\phi}{\phi_0} - 1\right)}$$

- Verma and Pruess (1988)

$$\frac{k - k_c}{k_0 - k_c} = \left(\frac{\phi - \phi_c}{\phi_0 - \phi_c}\right)^n$$

- Φ is ratio of pore to bulk volume

$$\phi = 1 - \frac{V_s\left(K_s, P, \tau'\right)}{V_0(1 - \epsilon_v)}$$

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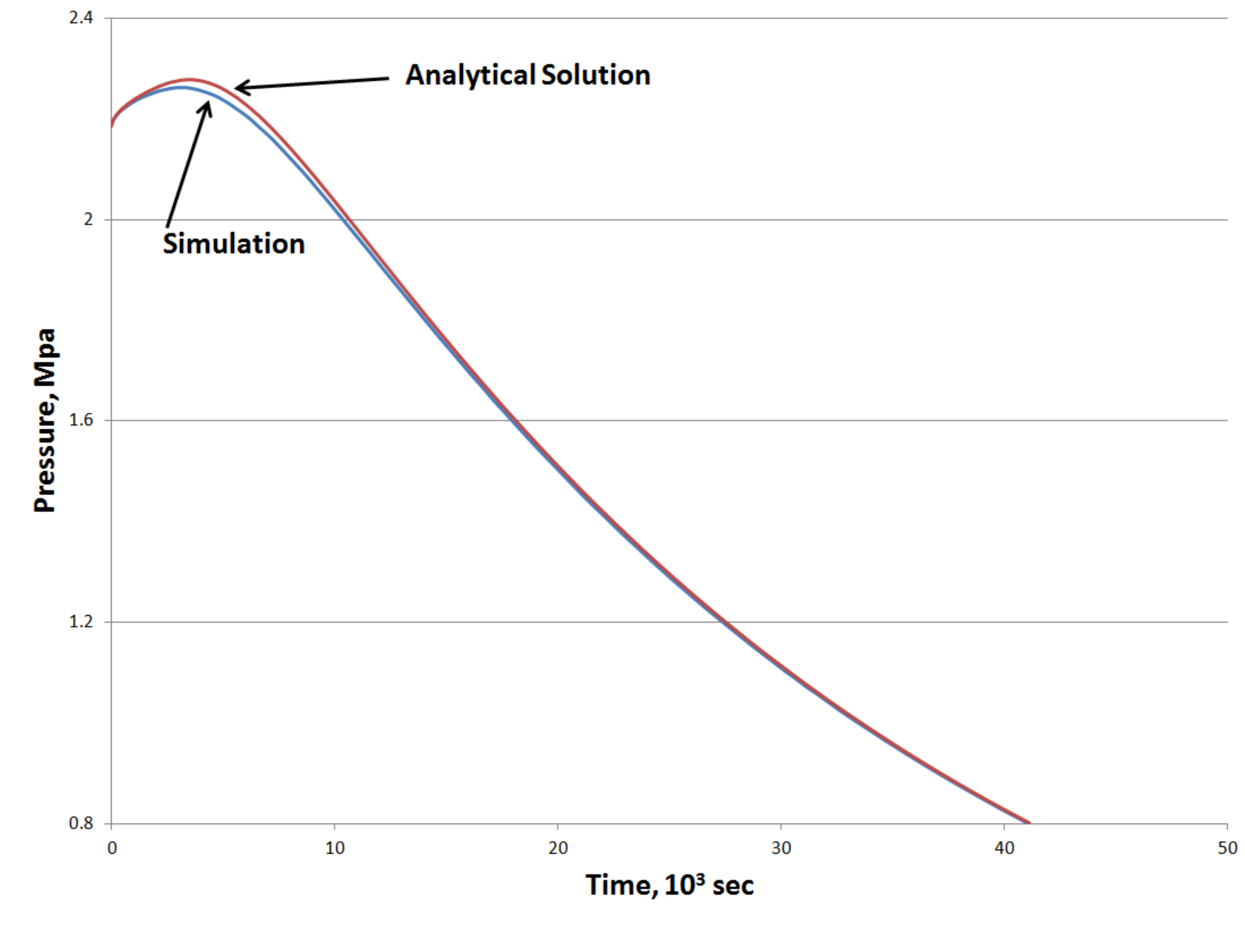
Mandel-Cryer Effect

- Poroelastic material, compressive force is applied to the top and bottom, allowed to drain laterally
- Instantaneous uniform pressure increase under undrained compression
- Pressure near the edges decreases from drainage
- Load transfer to center, causing further increase in center pressure to a maximum, then a decline
- Analytical solution: Abousleiman and Cheng (1996)

Mandel-Cryer Comparison



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3) Geochemical reactions between injected CO_2 and aquifer rock

- THMC simulator, fully coupled fluid and heat flow, geomechanics; fully/sequentially coupled geochemistry
- TOUGH2, TOUGHREACT formulation as starting point
- Geomechanics described by Mean Stress Equation
- Total chemical species = primary ones + secondary ones
- Number secondary = number independent reactions
- Secondary species include aqueous complexes, precipitates
- Solve transport equations for primary species only

Geochemical Reaction Formulation

- Reaction stoichiometry primary (j), secondary (i)

$$C_i = \sum_{j=1}^{N_c} v_{ij} C_j \qquad i = 1 \ldots N_R$$

- Aqueous complexes in equilibrium with primary species

$$c_i = K_i^{-1} \gamma_i^{-1} \prod_{j=1}^{N_c} c_j^{v_{ij}} \gamma_j^{v_{ij}}$$

- Equilibrium mineral dissolution:

$$\Omega_m = X_m^{-1} \lambda_m^{-1} K_m^{-1} \prod_{j=1}^{N_c} c_j^{v_{mj}} \gamma_j^{mj} \qquad m = 1 \ldots N_p \qquad SI_m = \mathrm{Log}\left(\Omega_m\right) = 0$$

- Kinetic mineral dissolution :

$$r_n = f\left(c_{1,} c_2, \ldots, c_{Nc}\right) = \pm k_n A_n \left|1 - \Omega_n^{\theta}\right|^{\eta} \qquad n = 1 \ldots N_q$$

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1D radial THMC model

- Conceptual model – 100m thick, 10,000 m radius
- Mineral composition in typical sandstone - quartz and oligoclase, feldspar, chlorite, illite
- Nine minerals initially present, eight produced later
- 16 kinetic chemical reactions
- Key chemical species Mg^{2+}, Na^{2+}, AlO_2^- , HCO_3^-
- 90 kg/s CO2 injected for 10 years
- Long term storage afterwards

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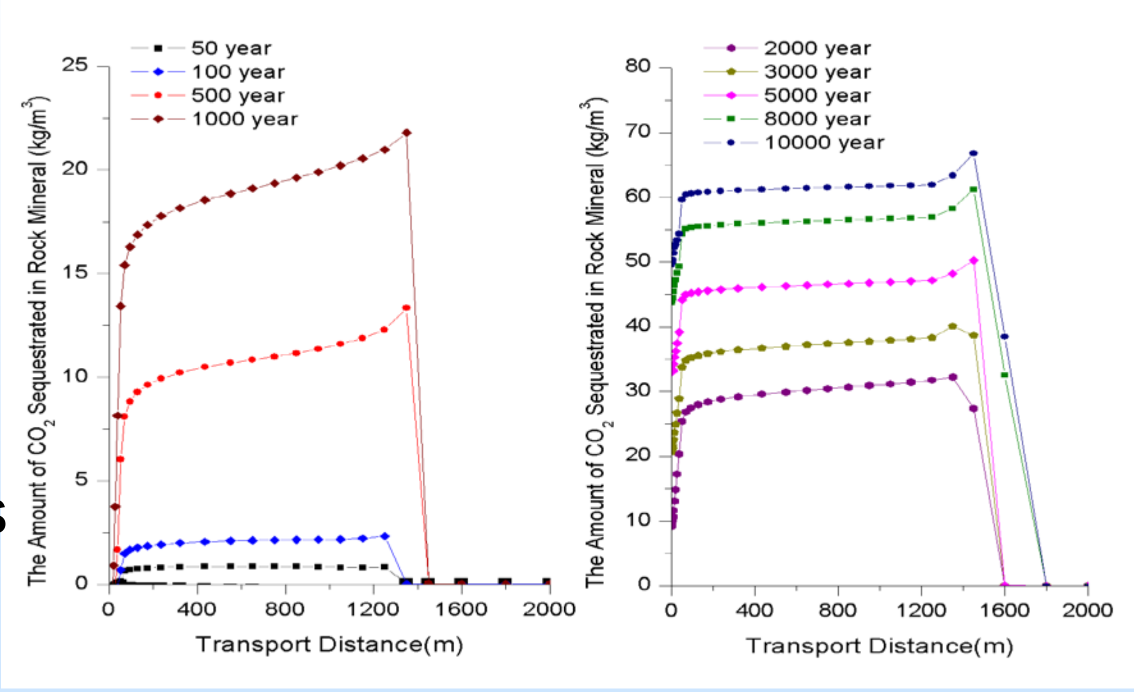
CO2 Sequestered in Minerals

- After 10 yrs injection – gaseous CO2 around injector, 2-phase area beyond, then single phase

- Gaseous CO2 dissolves in aqueous, increasing acidity and resulting in reactions



- CO2 precipitated as ankerite and dawsonite

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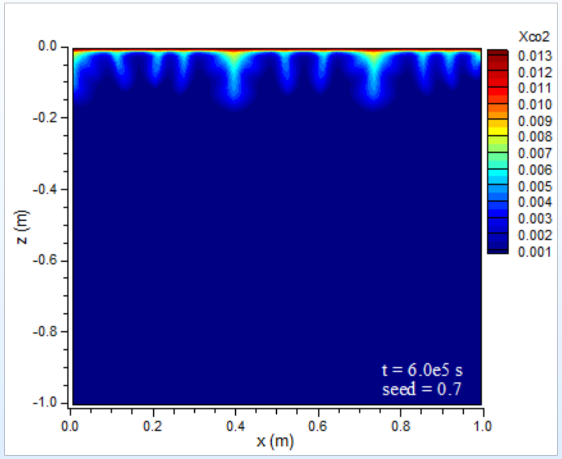
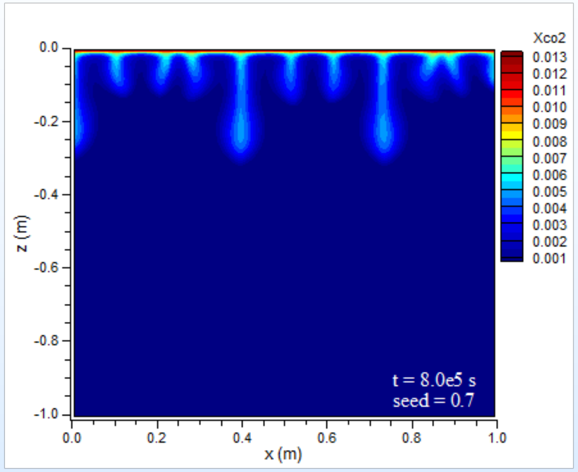
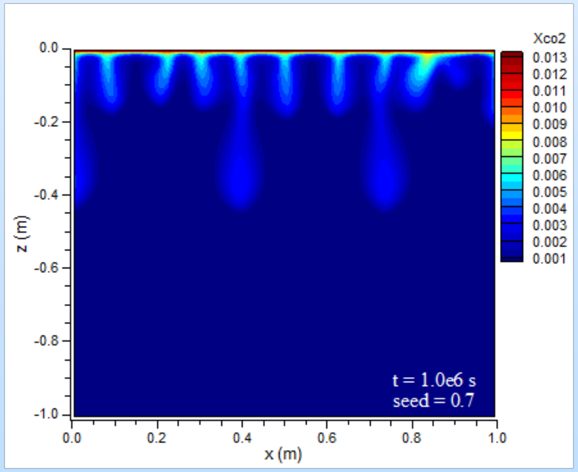
4) Modeling of density instability at CO_2-brine interface

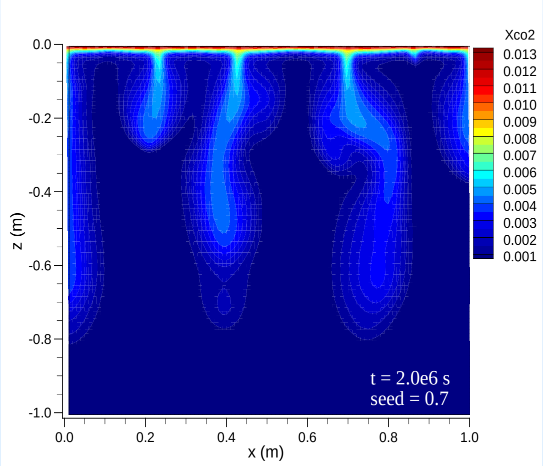
- 2D 100 × 100 grid, random permeability distribution about 10 D mean
- CO_2 diffuses through top of grid, fingers of dissolved CO_2 form there, grow, and reach bottom
- Several cases ran with different seeds that generate permeability heterogeneity
- Permeability distribution affects finger shape, but finger lengths are similar

Single Case, Varying Time









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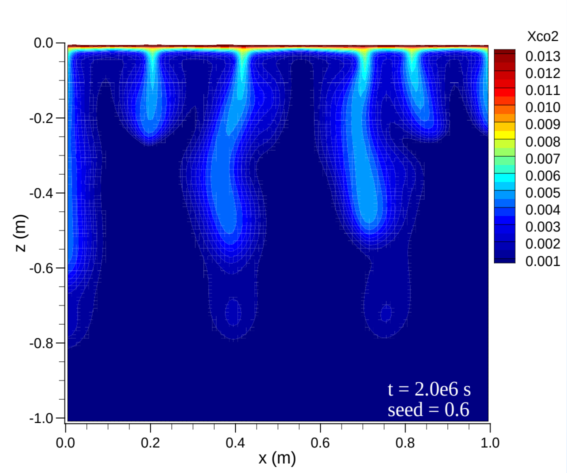
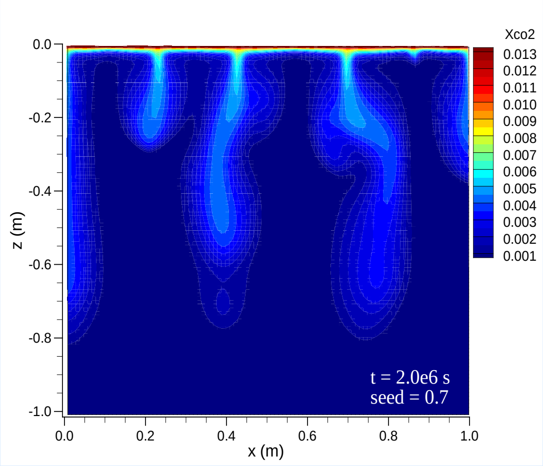
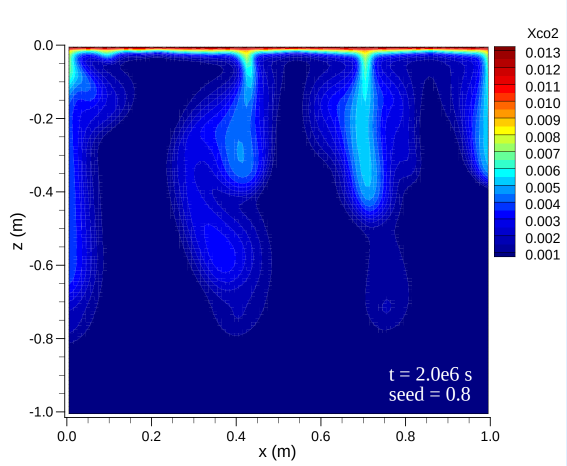
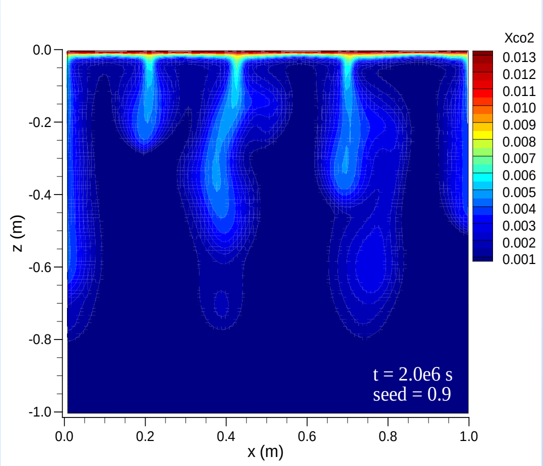
Constant Time, Various Cases









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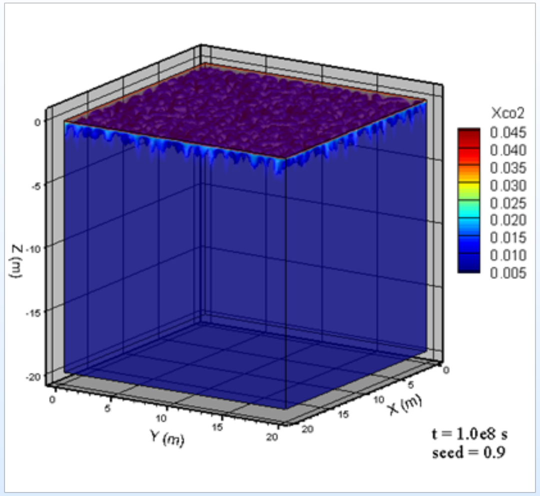
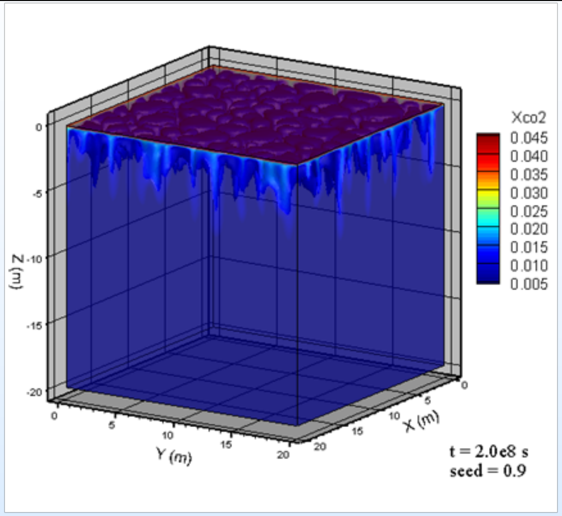
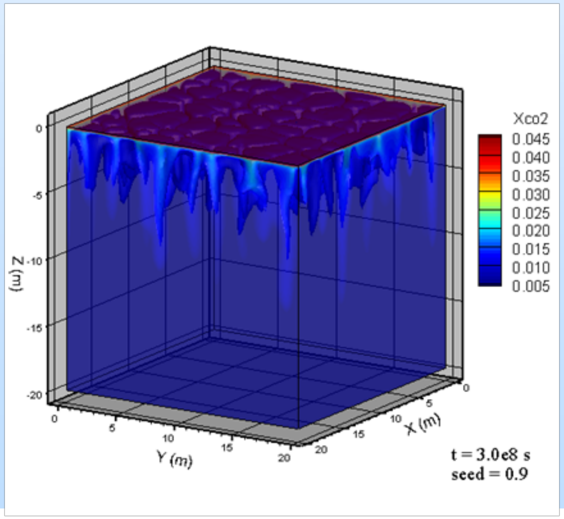
3D Simulations

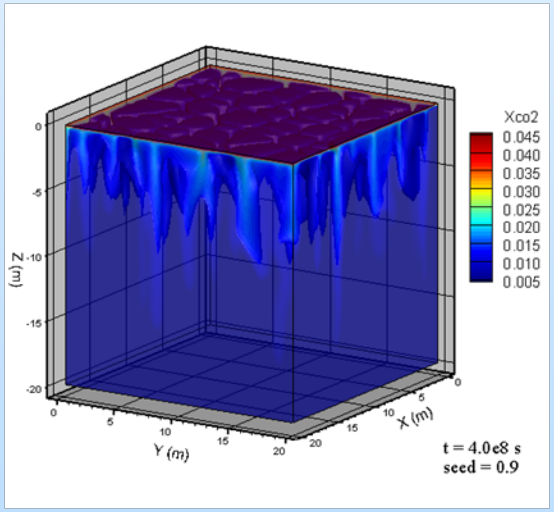
- 100 x 100 x 100 grid, 20 cm block length, random permeability distribution about 0.5 D mean
- CO2 diffuses through top of grid, fingers of dissolved CO2 form there, grow, and reach bottom
- Two cases ran with different seeds that generate permeability heterogeneity
- Early time fingers are uniform and cylindrical; later time ones are larger and flatter

3D Instability Simulation









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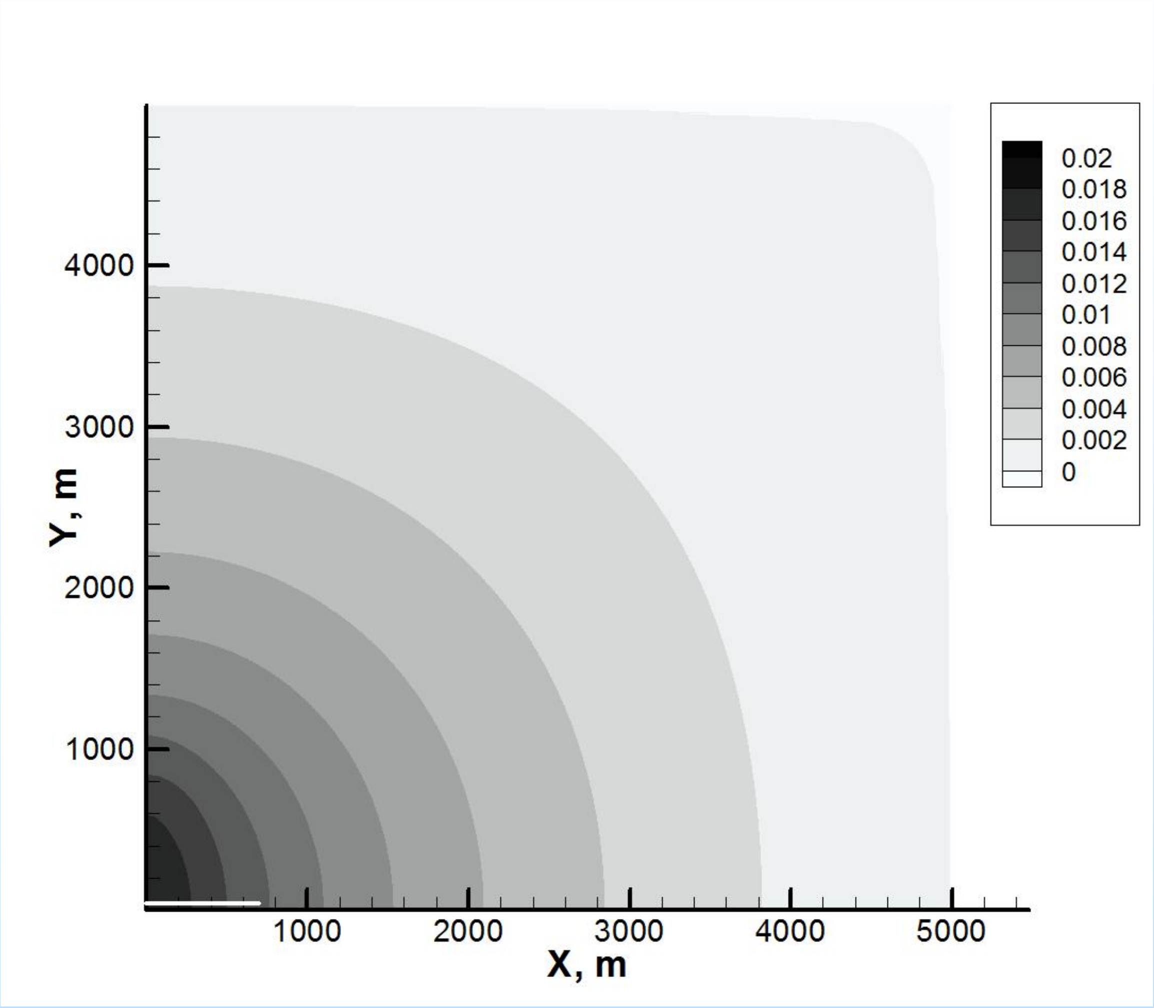
5) Development of efficient parallel computing algorithms

- TOUGH2-CSM written to to handle larger simulations (O[10^7-10^8] grid blocks) efficiently
- Cluster computer: 16 nodes, 16 processors/node (Intel ® 5260 2.4 GHz), 24 GB memory/node
- emgcluster upgrade: 16 additional nodes, 24 processors/node (Intel ® E5-2620 2.0 GHz), 32 GB memory/node; InfiniBand replaced Ethernet for inter-processor connections
- Upgraded cluster specifications: 32 nodes, 640 processors, 896 GB memory

In Salah Gas Project

- CO_2 injected into depleting gas field for storage
- Rutqvist et al. (2010): TOUGH2-FLAC simulation
- 10x10x4 km domain, 4 geological layers: Shallow Overburden, Caprock, Injection Zone, and Base
- 1.5 km horizontal injection well in center of Injection Zone, 13.6 kg/sec injected for three years
- TOUGH2-CSM simulation: (1/4) symmetry element (5x5x4 km),1000x1000x60 grid ($60 \cdot 10^6$ grid blocks)

In Salah Gas Project – Surface Uplift



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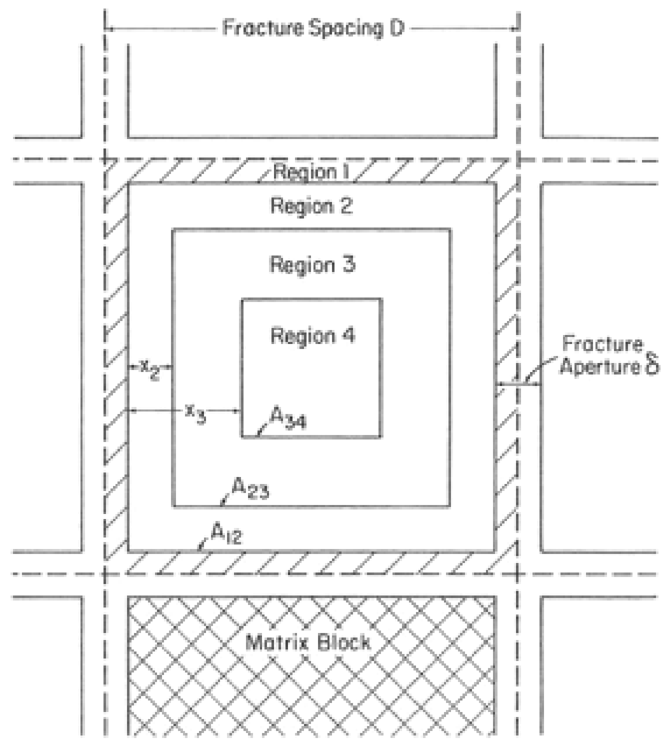
6) Development of general fracture conceptual models

- Fractured media simulated using MINC (multiple interacting continuum) model
- Variables associated with primary grid block: pressure, mass fractions, and temperature for each MINC block; mean stress common to all MINC blocks

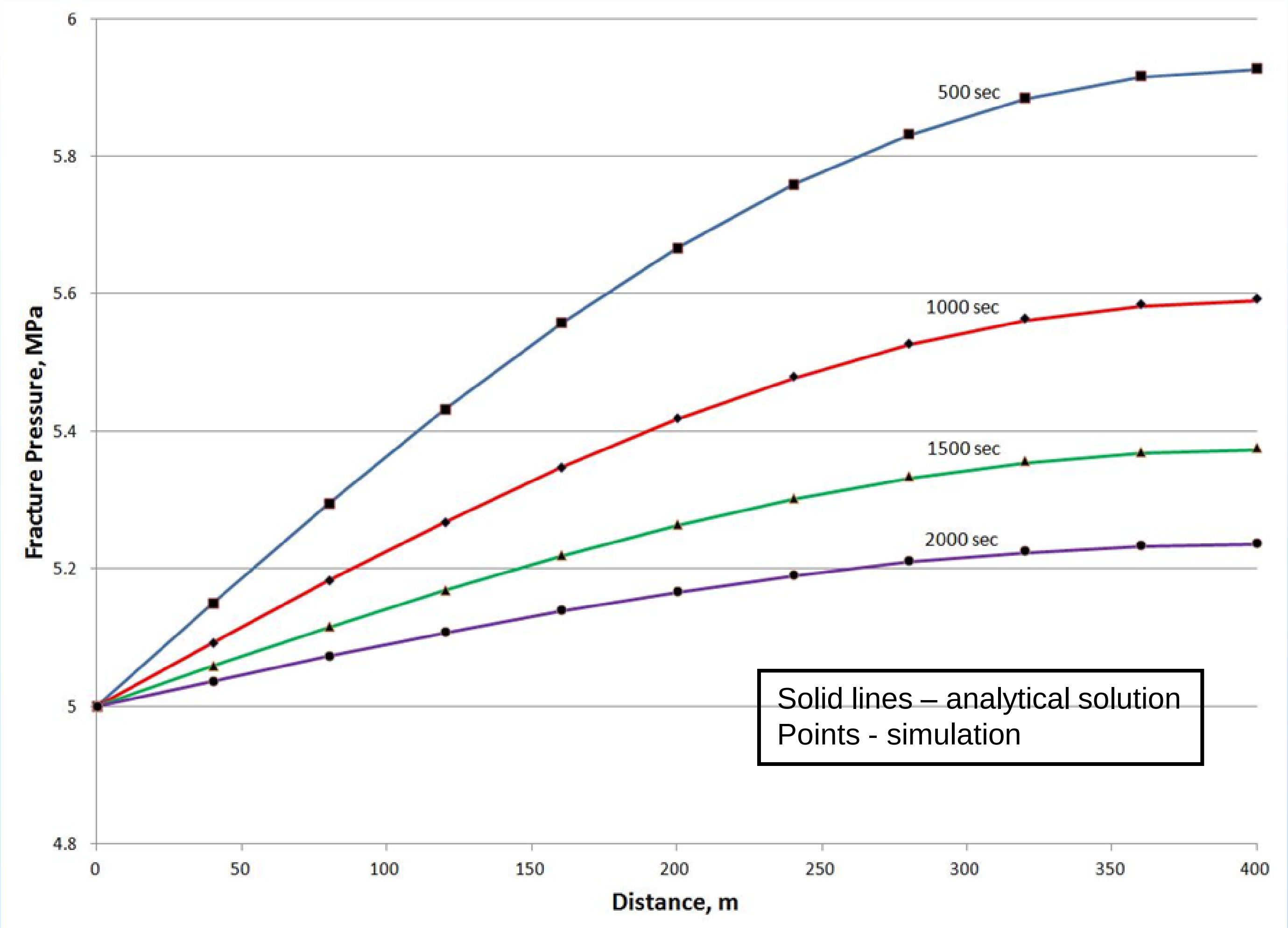


MINC partitioning of an idealized fracture system [Pruess, 1983]

1D Consolidation, Double Φ

- Apply load to top of fluid-filled double Φ column
- Load induces instantaneous deformation and pressure increase
- Fluid then drains out of column top and the pressure dissipates
- Analytical solution presented by Wilson and Aifantis (1982) with uniaxial strain and constant applied load

1D Consolidation Comparison



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TOUGH2-CSM Workshop

- June 5-6, 2013 at Colorado School of Mines
- Workshop topics were:
  - Mathematical model
  - Parallel code structure
  - Code installation, compilation and execution
  - Input and output file descriptions
  - Running sample problems
- 30 attendees - graduate students, researchers and professors from academia, and some from industry

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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
- Wrote fully coupled geochemical reaction model
- Studied and simulated density-driven instability
- Staged TOUGH2-CSM workshop to transfer technology to others

Summary

- Project is on schedule and on budget as planned
- Scheduled work is mostly completed
- Final report to be issued

Appendix

Organization Chart

Colorado School of Mines

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

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Gantt Chart

Figure 5.1: Milestone Status Report - Thick red line: Planned progress; Cells with dark grey: Actual progress

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

Publications

- Winterfeld, P. H., Wu, Y.-S., 2011, SPE 141514 - Parallel Simulation of CO2 Sequestration with Rock Deformation in Saline Aquifers, 2011 SPE Reservoir Simulation Symposium held 21-23 February, 2011, in The Woodlands, TX.
- Winterfeld, P. H., Wu, Y.-S., 2011, Numerical Simulation of CO2 Sequestration in Saline Aquifers with Geomechanical Effects,10th Annual Conference on Carbon Capture and Sequestration, May 2-5, 2011, in Pittsburgh, PA.
- Winterfeld, P. H., Wu, Y.-S., Pruess, K., Oldenburg, C., 2012, Development of Advanced Thermal-Hydrological-Mechanical Model for CO2 Storage in Porous and Fractured Saline Aquifers, TOUGH Symposium 2012.
- Zhang, R., Yin, X., Winterfeld, P. H., Wu, Y.-S.: A Fully Coupled Model of NonIsothermal Multiphase Flow, Geomechanics, and Chemistry During CO2 Sequestration in Brine Aquifers, TOUGH Symposium 2012.
- Zhang, R., Yin, X., Wu, Y.-S., Winterfeld, P. H., 2012, A Fully Coupled Model of Nonisothermal Multiphase Flow, Solute Transport and Reactive Chemistry in Porous Media, SPE Annual Technical Conference and Exhibition held in San Antonio, Texas, USA, 8-10 October 2012.

Publications, continued

- Winterfeld, P. H., Wu, Y.-S., 2012, A Novel Fully Coupled Geomechanical Model for CO_2 Sequestration in Fractured and Porous Brine Aquifers, XIX International Conference on Computational Methods in Water Resources (CMWR 2012).

- Winterfeld, P. H., Wu, Y.-S.: Chapter 8: Simulation of CO_2 Sequestration in Brine Aquifers with Geomechanical Coupling. Edited by Professor Jochen Bundschuh, Head of the Hydrogeology Unit at the University of Southern Queensland, Australia/Royal Institute of Technology, Sweden, and Rafid Al-Khoury, Senior Scientist at Delft University of Technology, in Computational Models for CO_2 Sequestration and Compressed Air Energy Storage, to be published by Taylor & Francis/CRC press.

- Winterfeld, P. H., Wu, Y.-S.: Development of Advanced Thermal-Hydrological-Mechanical Model for CO_2 Storage in Porous and Fractured Saline Aquifers, to be published in Computers and Geosciences