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

DE-FE0000988

Philip H. Winterfeld

Colorado School of Mines

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

August 12-14, 2014

Presentation Outline

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

COLORADOSCHOOLOFMINES
EARTH • ENERGY • ENVIRONMENT

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

COLORADOSCHOOLOFMINES
EARTH • ENERGY • ENVIRONMENT

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

Project Overview: Current Project Status

• Four-year project, October 1, 2009 – September 30, 2013

• Major project objectives were attained by September 30, 2013

• No-cost extension for period covering 1 October 2013 – 30 September 2014

• Three tasks: improvement of parallel computing schemes; additional validation and application of the model; improvement in documentation, publication and technology transfer

COLORADO SCHOOL OF MINES
EARTH • ENERGY • ENVIRONMENT

Technical Status

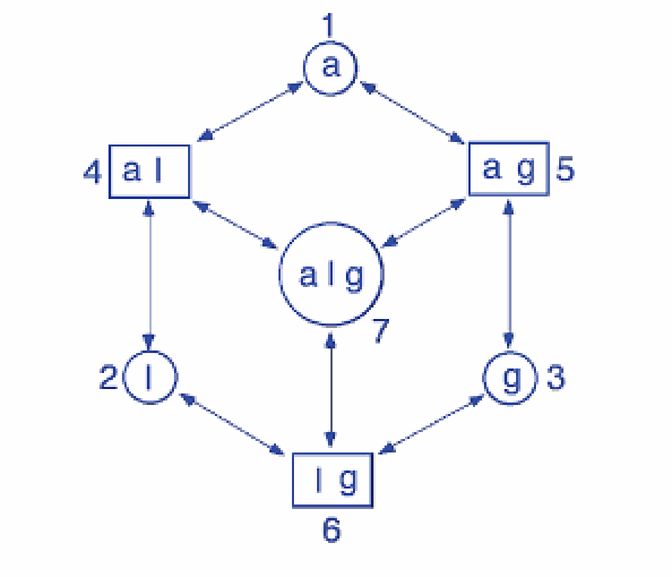
1) Three-phase non-isothermal module for CO_2-brine flow

- TOUGH2 fluid property module, part of TOUGH2 family of codes
- Called ECO2M, based on earlier ECO2N module, uses many of its fluid property correlations
- ECO2N does not distinguish between liquid and gaseous CO_2-rich phases; ECO2M does
- Developed code, wrote documentation (user's manual) for module, including test problems, tested code

COLORADOSCHOOLOFMINES
EARTH • ENERGY • ENVIRONMENT

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

- Developed for CO_2 sequestration, highly accurate for conditions of interest (10 - 110 °C, P < 600 bar)
- Three phases: aqueous (a), liquid CO_2-rich (l), gaseous CO_2-rich (g); plus two- and three-phase combinations
- Seven possible phase combinations, as shown



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

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

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

COLORADO SCHOOL OF MINES
EARTH • ENERGY • ENVIRONMENT

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)

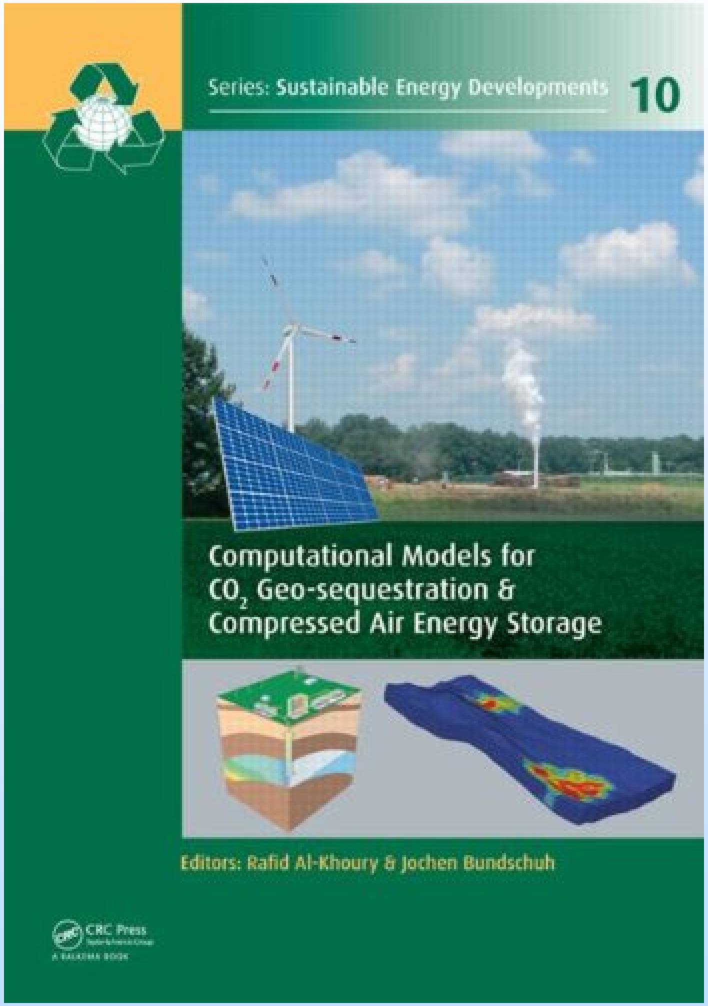
$$\frac{k - k_c}{k_0 - k_c} = \left(\frac{\phi - \phi_c}{\phi_0 - \phi_c}\right)^n$$

- Φ is ratio of pore to bulk volume

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

COLORADOSCHOOLOFMINES
EARTH • ENERGY • ENVIRONMENT

Book Chapter



COLORADOSCHOOLOFMINES
EARTH • ENERGY • ENVIRONMENT

Chapter 8

8. Simulation of CO2 sequestration in brine aquifers with geomechanical coupling

Philip H.Winterfeld &Yu-Shu Wu

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:

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

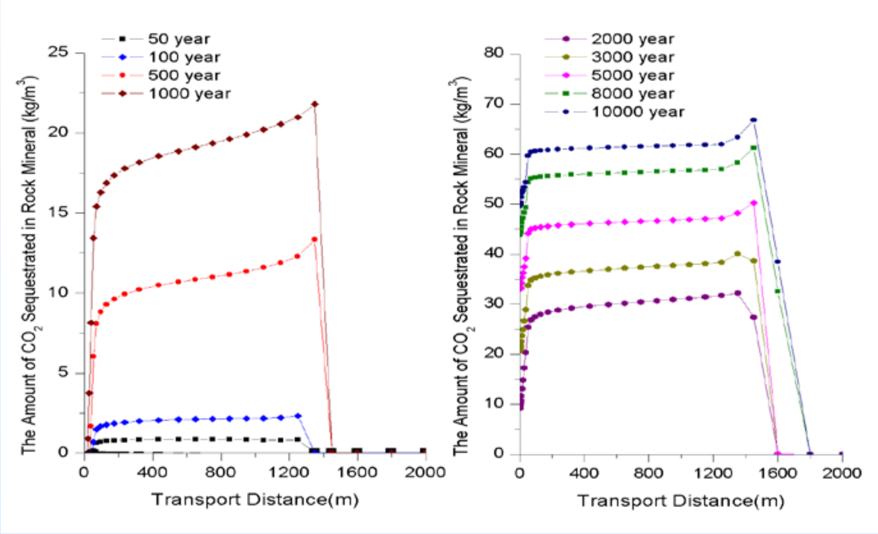
- Kinetic mineral dissolution :

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

COLORADOSCHOOLOFMINES
EARTH • ENERGY • ENVIRONMENT

1D Radial Conceptual THMC Model

- Mineral composition in typical sandstone
- 16 kinetic chemical reactions
- 90 kg/s CO2 injected for 10 years
- Long term storage afterwards



Ronglei Zhang, Ph.D.

- Petroleum Engineering, CSM, fall 2013
- B.S. and M.S., Petroleum Engineering, Northeast Petroleum University, China
- Thesis title: “Numerical Simulation of Thermal-Hydrological-Mechanical-Chemical Processes During CO2 Geo-Sequestration”
- Currently works for Chevron Energy Technology Company in Houston TX

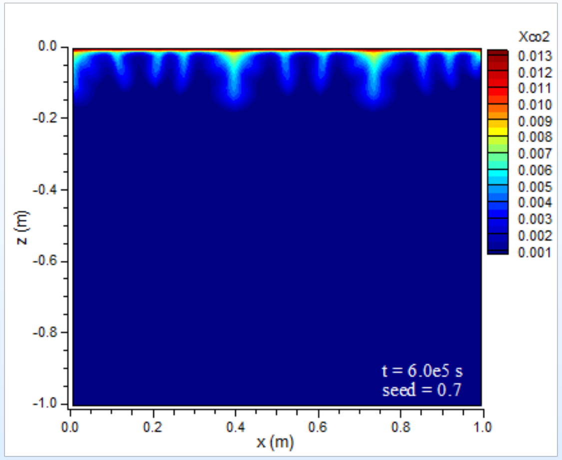
COLORADOSCHOOLOFMINES
EARTH • ENERGY • ENVIRONMENT

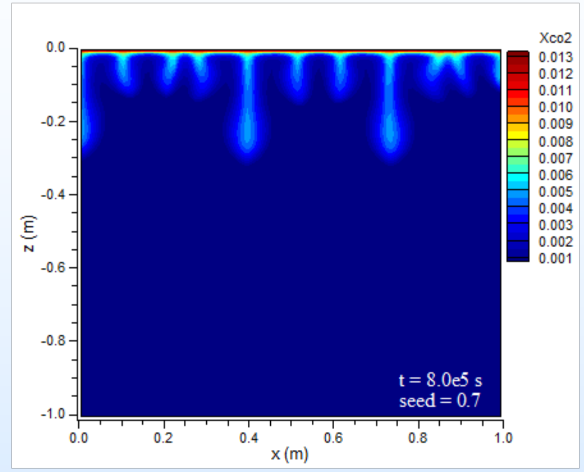
4) Modeling of density instability at CO_2-brine interface

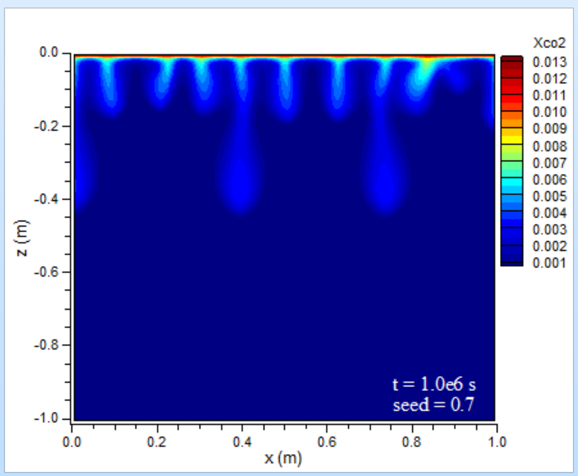
- 2D 100 × 100 grid, random permeability distribution about 10 D mean
- CO_2 diffuses through top of grid, fingers of dissolved CO_2 form there, grow, and reach bottom
- Several cases ran with different seeds that generate permeability heterogeneity
- Permeability distribution affects finger shape, but finger lengths are similar
- 3D simulations as well

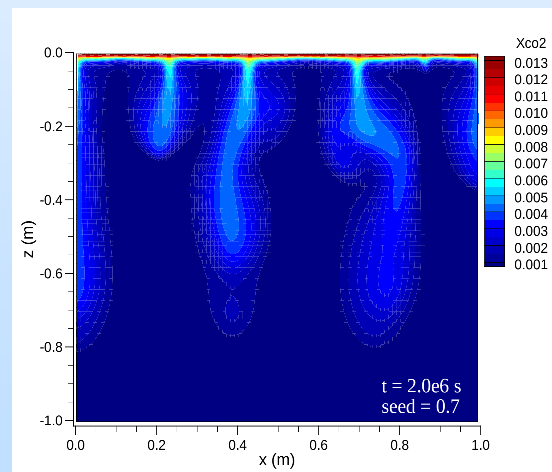
COLORADOSCHOOLOFMINES
EARTH • ENERGY • ENVIRONMENT

Single Case, Varying Time

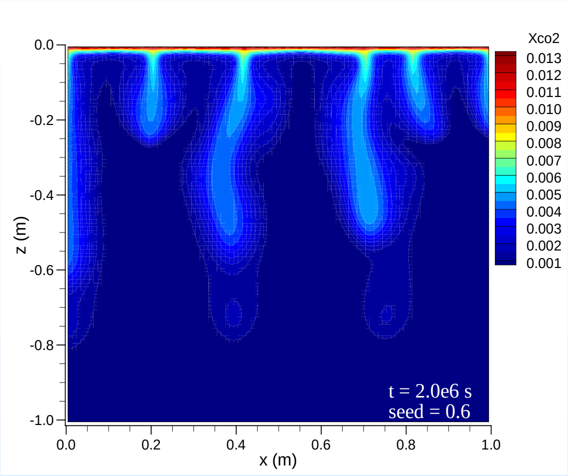


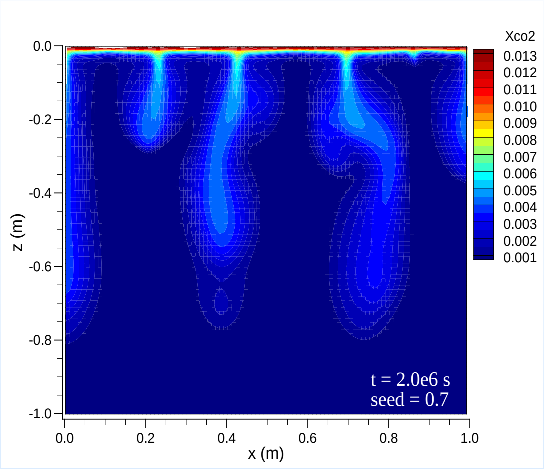


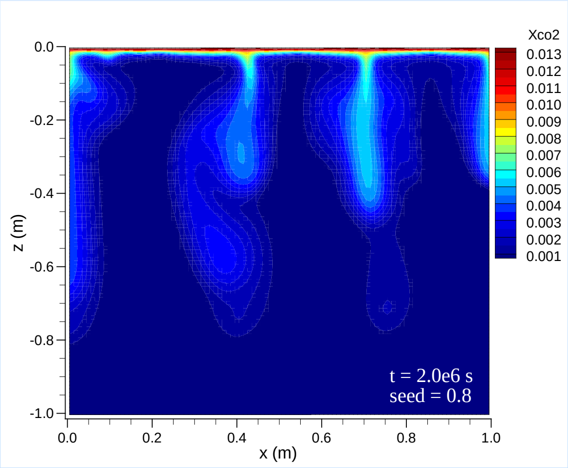


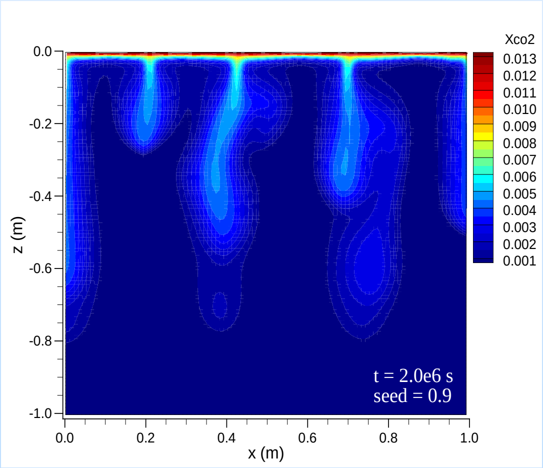


Constant Time, Various Cases







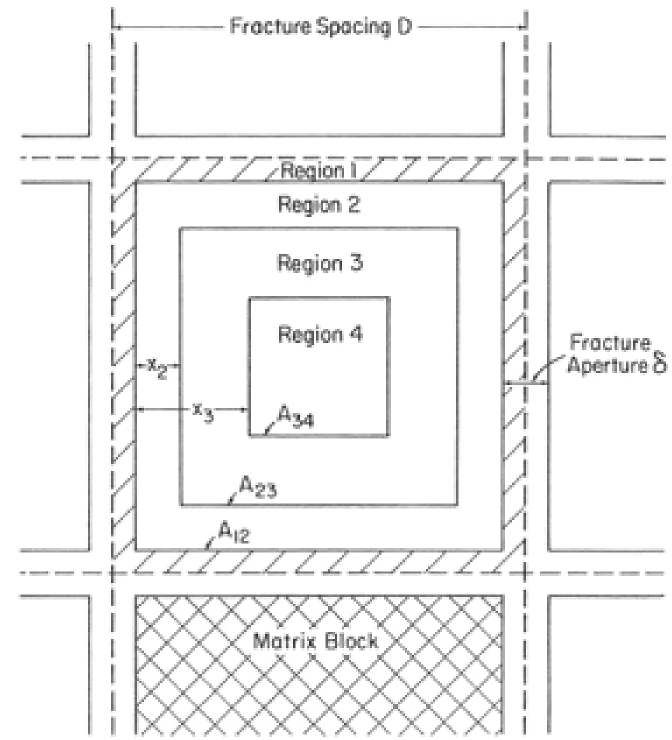


5) Development of efficient parallel computing algorithms

- Cluster computer called emgcluster
- Initially had 16 nodes with 16 processors/node (Intel ® 5260 2.4 GHz), 24 GB memory/node)
- Cluster upgraded 8/13
- Additional 16 nodes with 24 processors/node (Intel ® E5-2620 2.0 GHz), 32 GB memory/node
- InfiniBand for inter-processor connections

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]

COLORADO SCHOOL OF MINES
EARTH • ENERGY • ENVIRONMENT

1D Consolidation Simulation, Compression

- Initial unstrained state: $P_0 = \tau_{m,0}$
- Mean stress $\tau_{m,1}$ applied at top to induces pressure P_1
- For uniaxial deformation

$$\tau_m = \frac{1}{3}\frac{(1+\nu)}{(1-\nu)}(\tau_{zz} - \alpha P) + \alpha P$$

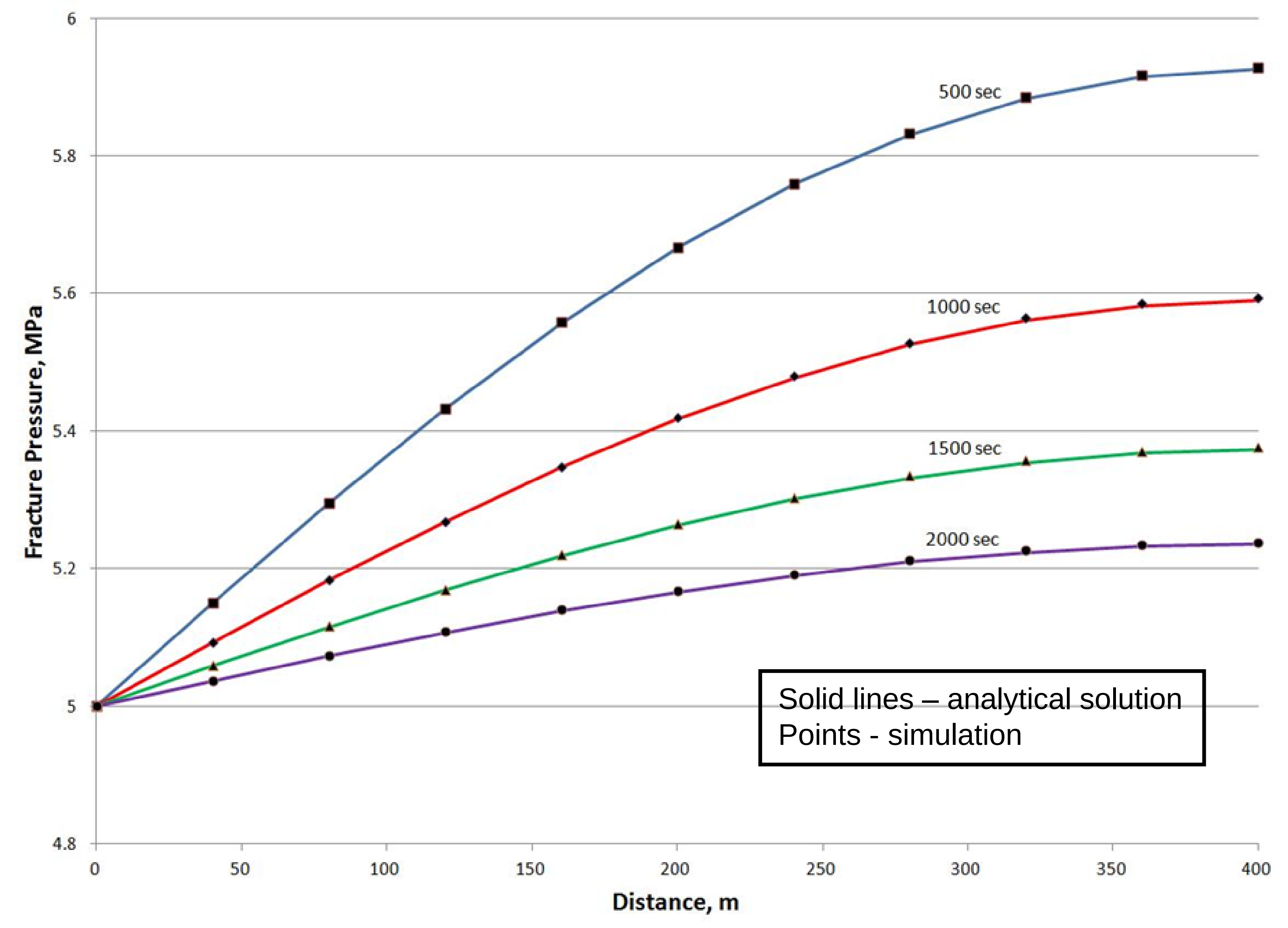
which is used to calculate applied load $\tau_{zz,1}$ from $\tau_{m,1}$ and P_1

COLORADOSCHOOLOFMINES
EARTH • ENERGY • ENVIRONMENT

1D Consolidation Simulation, Drainage

- Start at uniform mean stress $\tau_{m,1}$ and pressure P_1
- Impose initial pressure P_0 at top
- Mean stress imposed at top, $\tau_{m,2}$, calculated from P_0 and constant applied z-direction stress, $\tau_{zz,1}$
- Fluid drains from top until pressure in the column relaxes to the initial value P_0

1D Consolidation Comparison



"Parallel Fully-Coupled Hydromechanical Modeling of CO2 Leakage Through Fluid-Driven Fracture Zones During Injection," by Z. Huang, P. H. Winterfeld, and Y.-S. Wu

- Prediction of rock fracturing pressure based on stress field and pore pressure
- Correlations of hydraulic properties with stress
- Assumptions that yield stress components from mean stress
- Simulator verification using analytical solutions
- Fluid flow with natural system failures, conclusions include transient pressure response from vertical pathways created by CO2 injection can be detected by PDG's and there are strong correlations between leakage and monitoring pressure

Code and User Manuals

- User manuals are being proofread, edited, and updated
- Code will be released and will meet the standards for public code, such as documentation and readability
- Efficiency of code will be enhanced where possible

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 October, 2014

COLORADOSCHOOLOFMINES
EARTH • ENERGY • ENVIRONMENT

Appendix

Organization Chart

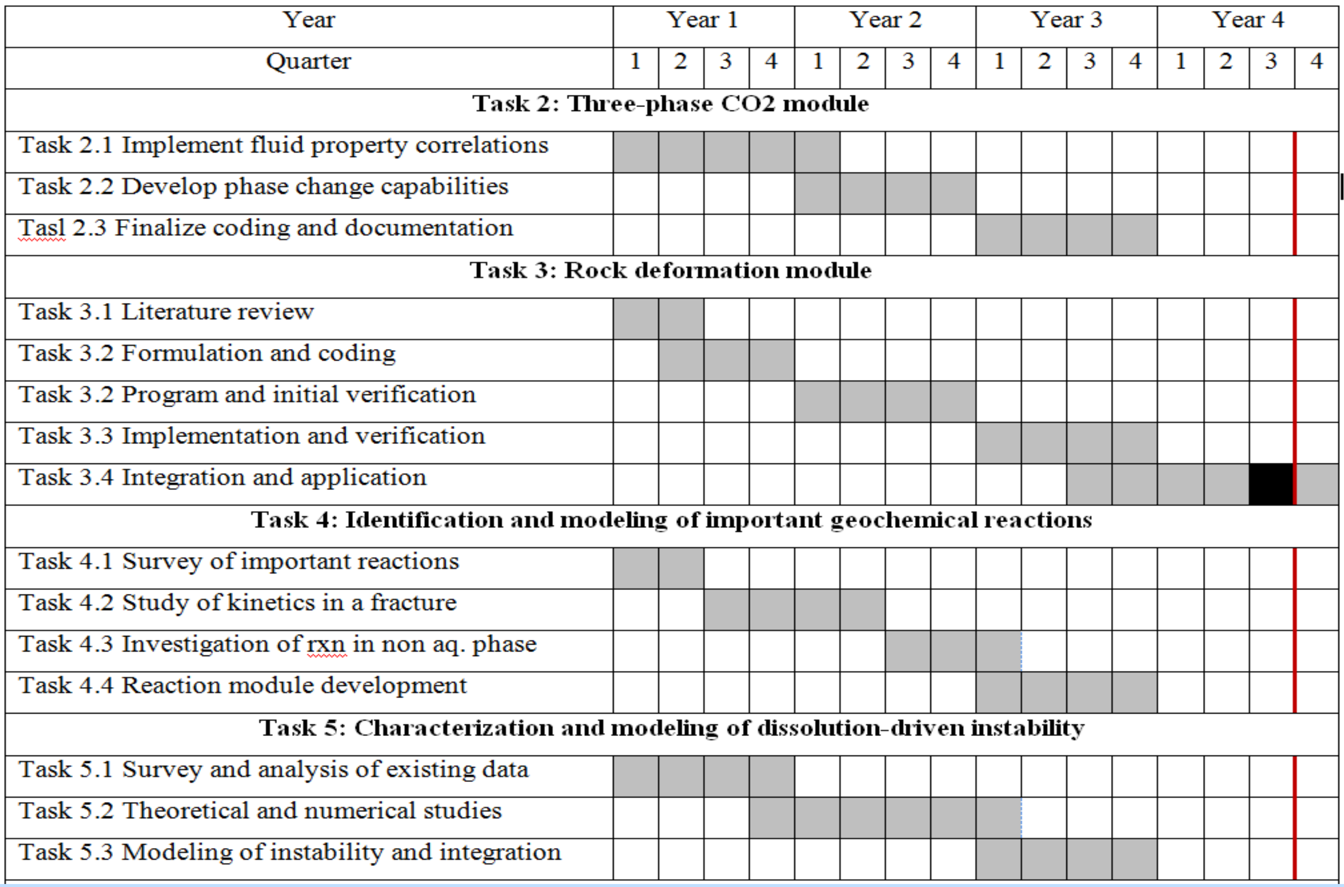
<u>Colorado School of Mines</u>
Philip Winterfeld, Research Associate Professor, Petroleum Eng.
Yu-Shu Wu, Prof. and CMG Reservoir Modeling Chair, Pet. Eng.
Xiaolong Yin, Assistant Professor, Petroleum Engineering
Ronglei Zhang, Ph.D. Candidate, Petroleum Engineering

<u>Computer Modeling Group</u>
(CMG)
Industry sponsor

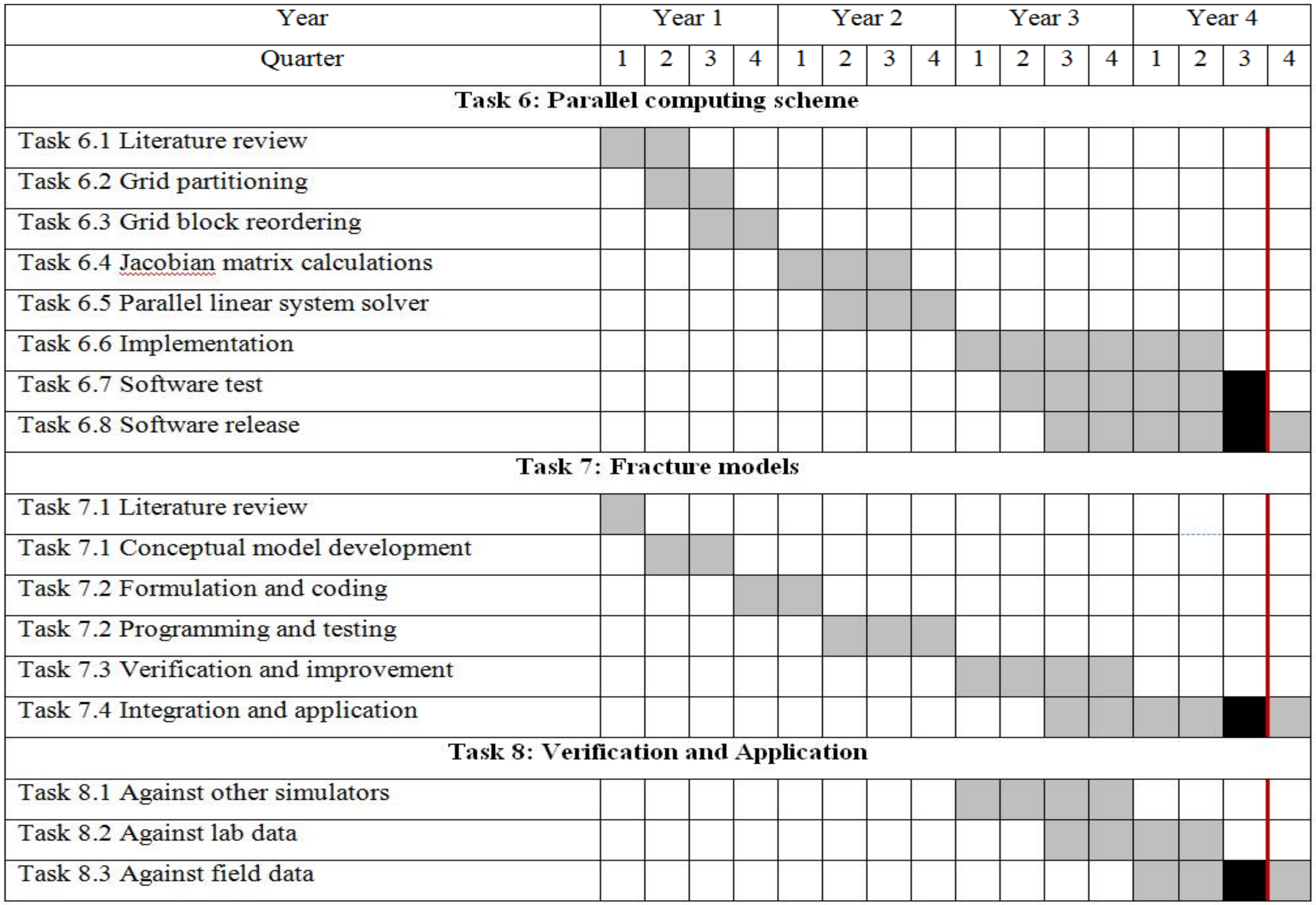
<u>Lawrence Berkeley National Laboratory</u>
Karsten Pruess, Senior Scientist, Hydrogeology (retired)
Curt Oldenburg, Staff Geological Scientist and Head Geologic Carbon Sequestration Program, Hydrogeology

Gantt Chart

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



Gantt Chart,Cont’d



Publications

- Huang, Z., Winterfeld, P. H., Wu, Y.-S. : “Parallel Fully-Coupled Hydromechanical Modeling of CO2 Leakage Through Fluid-Driven Fracture Zones During Injection,” submitted to International Journal of Green House Gas Control
- 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.

Publications, continued

- 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.
- Winterfeld, P. H., Wu, Y.-S., 2012, A Novel Fully Coupled Geomechanical Model for CO2 Sequestration in Fractured and Porous Brine Aquifers, XIX International Conference on Computational Methods in Water Resources (CMWR 2012).
- Winterfeld, P.H. and Y.S. Wu, "Simulation of CO2 sequestration in brine aquifers with geomechanical coupling," in "*Computational Models for CO2 Sequestration and Compressed Air Energy Storage*," chapter 8, edited by J. Bundschuh and R. Al-Khoury, CRC Press, 2014
- Wu, Y.-S. , Xiong, Y., Zhang, R., Winterfeld, P. H.: "Simulation of Coupled Thermal–Hydrological–Mechanical–Chemical (THMC) Processes in Porous Media," presented at the XX International Conference on Computational Methods in Water Resources (CMWR 2014), June 10-13, 2014, at the University of Stuttgart, Germany

COLORADOSCHOOLOFMINES
EARTH • ENERGY • ENVIRONMENT