Numerical Simulation of CO_2 Storage in Saline Aquifers

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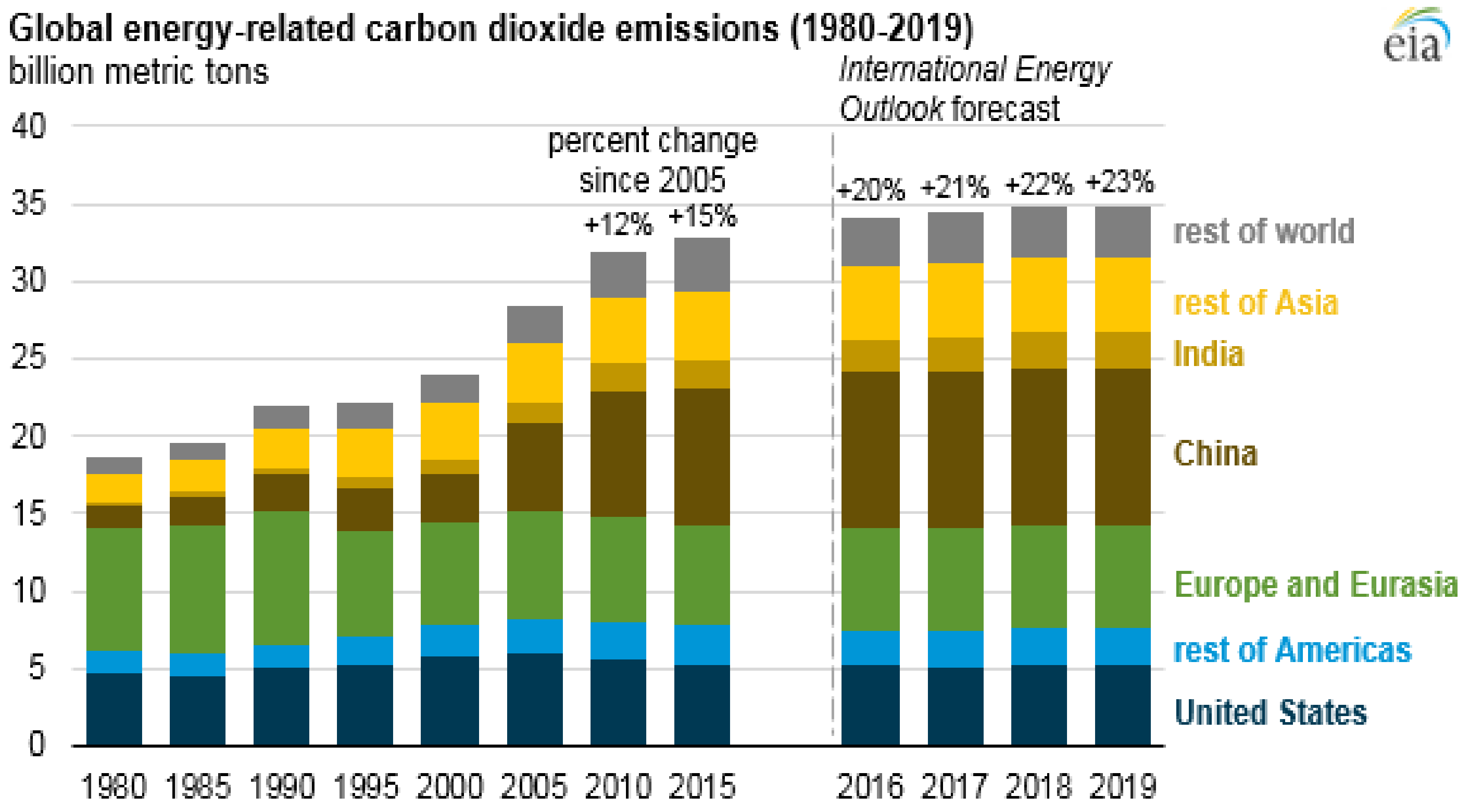
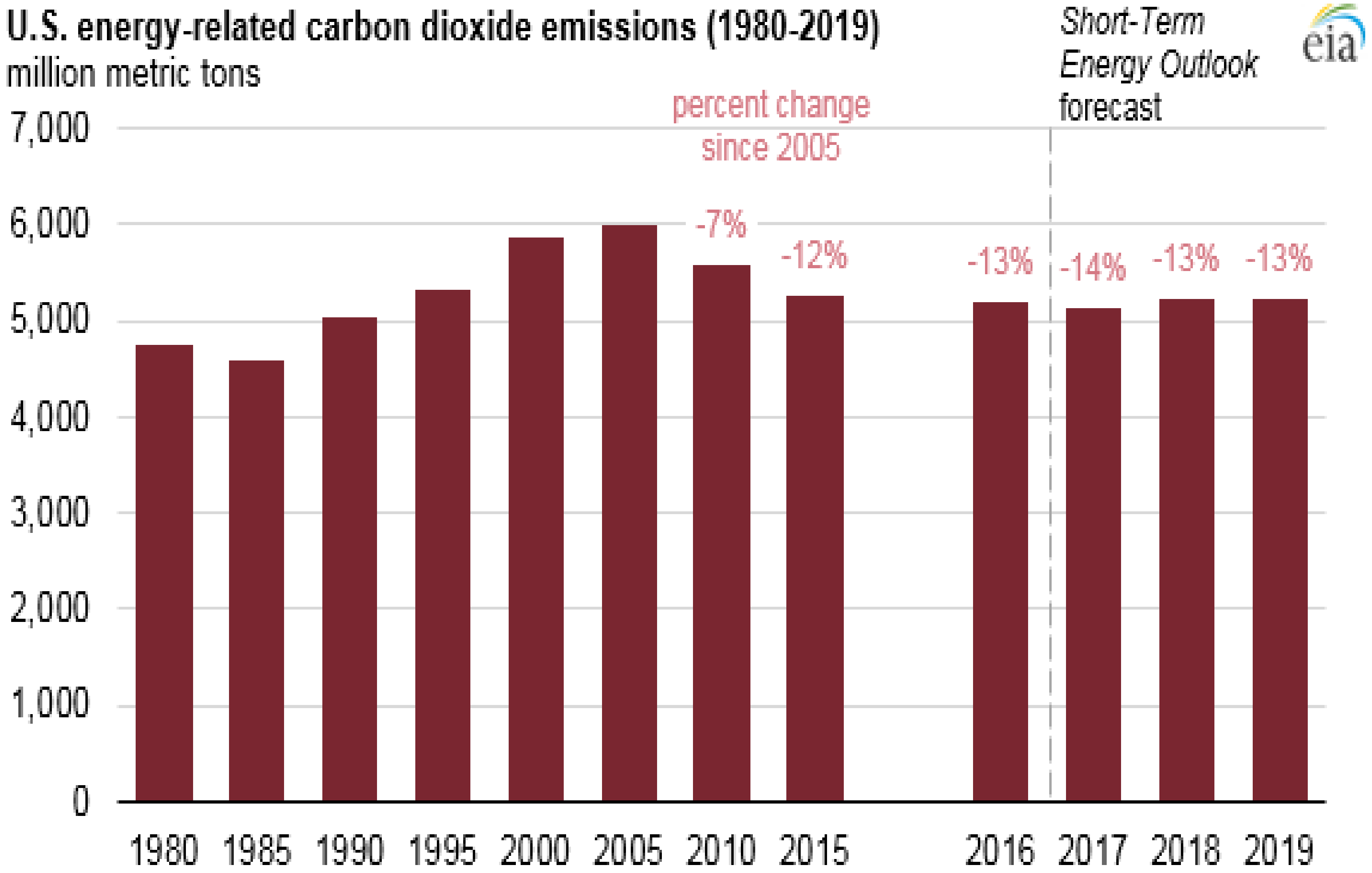
Outline

1. Background
2. Physical processes
3. TOUGH2-CSM
4. Technical approaches
5. Rock deformation and Geomechnics
6. Simulation examples
7. Concluding remarks

Near Future Challenges

- Global CO_2 emissions



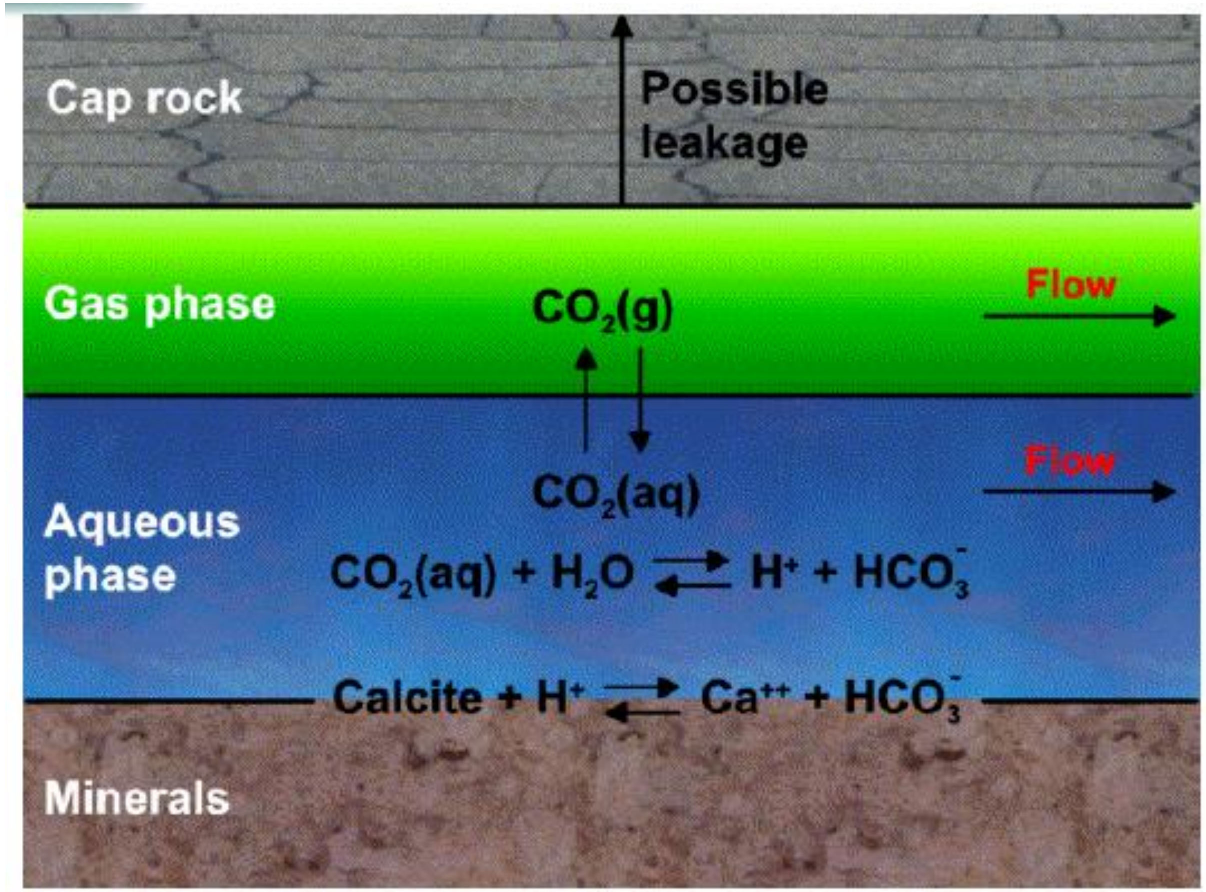

U.S. energy-related carbon dioxide emissions (1980-2019)
million metric tons
Short-Term
Energy Outlook
forecast
eia
percent change
since 2005
7,000
6,000
5,000
4,000
3,000
2,000
1,000
0
-7%
-12%
-13%
-14%
-13%
-13%
1980
1985
1990
1995
2000
2005
2010
2015
2016
2017
2018
2019

Physical Processes

Structural Integrity – Elevated pressure and effects on existing fractures / faults

Dissolution – Mass transfer between CO2 and formation brine

Geochemistry – Reactions induced by dissolved CO2 with aquifer rock (mineralization)



TOUGH2_CSM: CO_2 Sequestration Model

under development at Colorado School of Mines (CSM)

TOUGH2-CSM has been developed under 2 DOE funded projects:

Yu-Shu Wu (PI); Co-PI's: Xiaolong Yin and H. Kazemi (Colorado School of Mines); and Karsten Pruess and Curt Oldenburg**):** "Simulation of Coupled Processes of Flow, Transport and Storage of CO2 in Saline Aquifers," funded by the US DOE, 2009-2014

Yu-Shu Wu (PI); Co-PI's: Xiaolong Yin and Phil Winterfeld (Colorado School of Mines); and Tim Kneafsey and Jonny Rutqvist (Lawrence Berkeley National Laboratory), 3-Year Project: "Quantitative Characterization of Impacts of Coupled Geomechanics and Flow on Safe and Permanent Geological Storage of CO2 in Fractured Reservoirs," funded by the US Department of Energy, 2014-2018

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Technical Approaches of TOUGH2-CSM

- Based on TOUGH2-MP/ECO2N
- Numerical model: Integrated finite difference method
- H_2O-NaCl-CO_2 properties from ECO2N module
- ECO2M – new three-phase flow module
- CO_2 flow, transport and storage in saline aquifers
- Geomechanical processes occurring during CO_2 injection and storage
- Coupling geochemical reactions
- Parallel simulation
- General fracture conceptual model

General Framework Model

Mass Balance

for Component κ

$$M^{\kappa} = \sum_{\beta} \phi S_{\beta} \rho_{\beta} X_{\beta}^{\kappa} + R^{\kappa}$$

$$G^{k} = \lambda_{k} \left(\phi \sum_{\beta} \left(\rho_{\beta} S_{\beta} X_{\beta}^{k} \right) + R_{\beta}^{k} \right)$$

$$F^{k} = -\sum_{\beta} \nabla \bullet \left(\rho_{\beta} X_{\beta}^{k} \mathbf{v}_{\beta} \right) + \sum_{\beta} \nabla \bullet \left(\underline{D}_{\beta}^{k} \bullet \nabla \left(\rho_{\beta} X_{\beta}^{k} \right) \right)$$

Energy Balance

$$M^{h} = (1-\phi)\rho_{R} C_{R} T + \phi \sum_{\beta} S_{\beta} \rho_{\beta} u_{\beta}$$

$$F^{h} = -\left[(1-\phi) K_{R} + \phi \sum_{\beta} S_{\beta} K_{\beta} \right] \nabla T + \sum_{\beta} h_{\beta} F_{\beta}$$

Stress Equilibrium

$$M = 0$$

$$F_{j} = \left[\Delta\sigma_{1j} \quad \Delta\sigma_{2j} \quad \Delta\sigma_{3j} \right]^{T}$$

$$\Delta\sigma_{ij} = 2G\varepsilon_{ij} + \delta_{ij} \lambda \varepsilon_{v} + 3\delta_{ij} \beta K \Delta T + \delta_{ij} \alpha \Delta P$$

$$\frac{d}{dt} \int_{V_n} \mathbf{M}^{\kappa} dV_n = \int_{\Gamma_n} \mathbf{F}^{\kappa} \bullet \mathbf{n} d\Gamma_n + \int_{V_n} G^{\kappa} dV_n + \int_{V_n} q^{\kappa} dV_n$$

TOUGH2-CSM-Geomechanics

- Fully coupled simulator for modeling THM effects in fractured and porous media saline aquifers
- Based on TOUGH2-MP fluid and heat flow formulation
- Geomechanics modeled with Mean Stress Equation plus stress tensor component equations
- Porosity and permeability depend on stress
- Rock failure scenarios including Mohr-Coulomb and tensile failure

Mean Stress Equation

- Hooke's law for a thermo-multi-poroelastic medium + stress equilibrium equation + strain tensor definition = Navier equation, then take divergence

$$\nabla \cdot \left[\frac{3(1-\upsilon)}{1+\upsilon} \nabla \tau_m + \mathbf{F}_b - \frac{2(1-2\upsilon)}{1+\upsilon} \nabla \left(\sum_j \left(\alpha_j P_j + 3\beta K \omega_j T_j \right) \right) \right] = 0$$

- Trace of Hooke's law: volumetric strain equation

$$K \varepsilon_v = \tau_m - \sum_j \left(\alpha_j P_j + 3\beta K \omega_j \left(T_j - T_{ref} \right) \right)$$

Stress Tensor Components

- Derivatives of thermo-multi-poroelastic Navier equation vector components are zero and yield equations for stress tensor components:

- Normal stresses:

$$\frac{\partial^2}{\partial x^2}\left[h(\mathbf{P},\mathbf{T})\right]+\frac{3}{2(1+\upsilon)}\frac{\partial^2}{\partial x^2}\left[\tau_m-h(\mathbf{P},\mathbf{T})\right]+$$

$$\frac{1}{2}\nabla^2\left[\tau_{xx}-h(\mathbf{P},\mathbf{T})-\frac{3\upsilon}{1+\upsilon}\left(\tau_m-h(\mathbf{P},\mathbf{T})\right)\right]+\frac{\partial F_{b,\mathrm{x}}}{\partial x}=0$$

- Shear stresses:

$$\frac{\partial^2}{\partial x\partial y}\left[h(\mathbf{P},\mathbf{T})\right]+\frac{3}{2(1+\upsilon)}\frac{\partial^2}{\partial x\partial y}\left[\tau_m-h(\mathbf{P},\mathbf{T})\right]+\frac{1}{2}\nabla^2\tau_{xy}+$$

$$\frac{1}{2}\left(\frac{\partial F_{b,\mathrm{y}}}{\partial x}+\frac{\partial F_{b,\mathrm{x}}}{\partial y}\right)=0$$

Solution of Equations

- Uses fully implicit integral finite difference method
- Mean stress variables (P,X,T,τ_m) solved for first
- Stress components (SC) then calculated
- SC depend only on mean stress variables
- SC Jacobian is 1x1; fast SC calculation; easily implemented

2D Cylindrical Coordinates

- zz- stress calculated as in Cartesian case
- Sum of strains:

$$\varepsilon_{rr} + \varepsilon_{\theta\theta} = \varepsilon_v - \varepsilon_{zz} = \frac{\partial u_r}{\partial r} + \frac{u_r}{r} = \frac{1}{r}\frac{\partial}{\partial r}\left(r u_r\right)$$

- Solve for displacement vector r-component:

$$u_r\left(r,z\right) = \frac{1}{r}\int_{r_0}^{r} \xi\left(\varepsilon_v\left(\xi,z\right) - \varepsilon_{zz}\left(\xi,z\right)\right) d\xi$$

- Strains: $\varepsilon_{\theta\theta} = \frac{u_r}{r}$; $\varepsilon_{rr} = \varepsilon_v - \varepsilon_{zz} - \varepsilon_{\theta\theta}$
- rθ shear stress calculated also

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

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

Rock Failure Modes

- Mohr-Coulomb failure – shear failure of fault

$$\tau > \mu\sigma' + C_0$$

- Mohr-Coulomb failure – shear failure of randomly fractured caprock

$$\sigma_1' > 3\sigma_3'$$

- Hydraulic fracturing due to pore pressure greater than minimum principal stress

$$P > \sigma_{\min} + \sigma_{tens}$$

Post Rock Failure

- Permeability and porosity correlated to stress for faults
- Fractured media – fracture aperture correlated to permeability:

$$k_f = \frac{bf}{12} \qquad b_f = b_f\left(\boldsymbol{\tau}'\right) \qquad \phi_f = \phi_f\left(\boldsymbol{\tau}'\right)$$

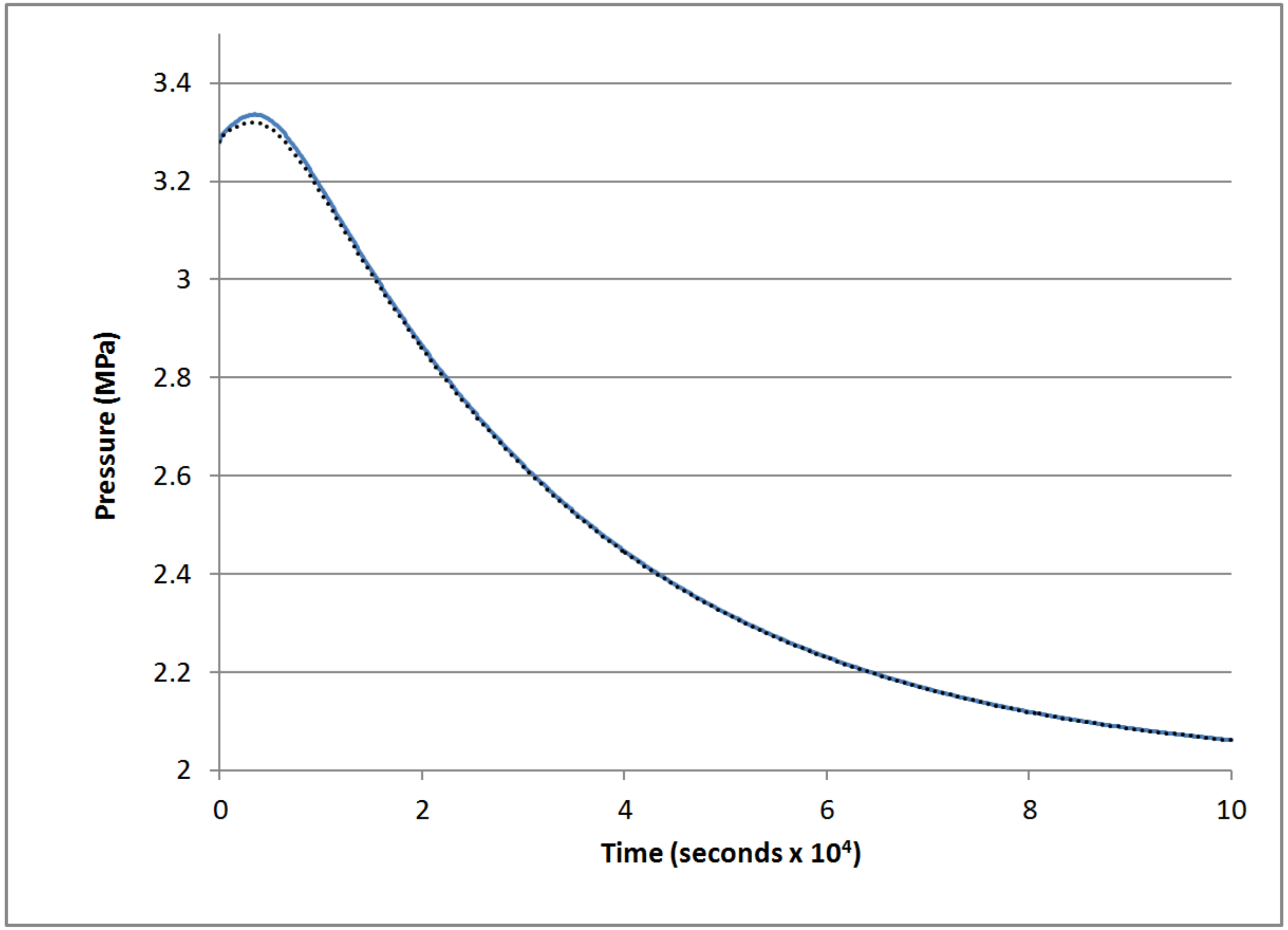
- Fracture growth and extension (stress intensity factor):

$$K_I > K_{IC} \qquad d \approx \left(\frac{K_I - K_{IC}}{K_{IC}}\right)^n$$

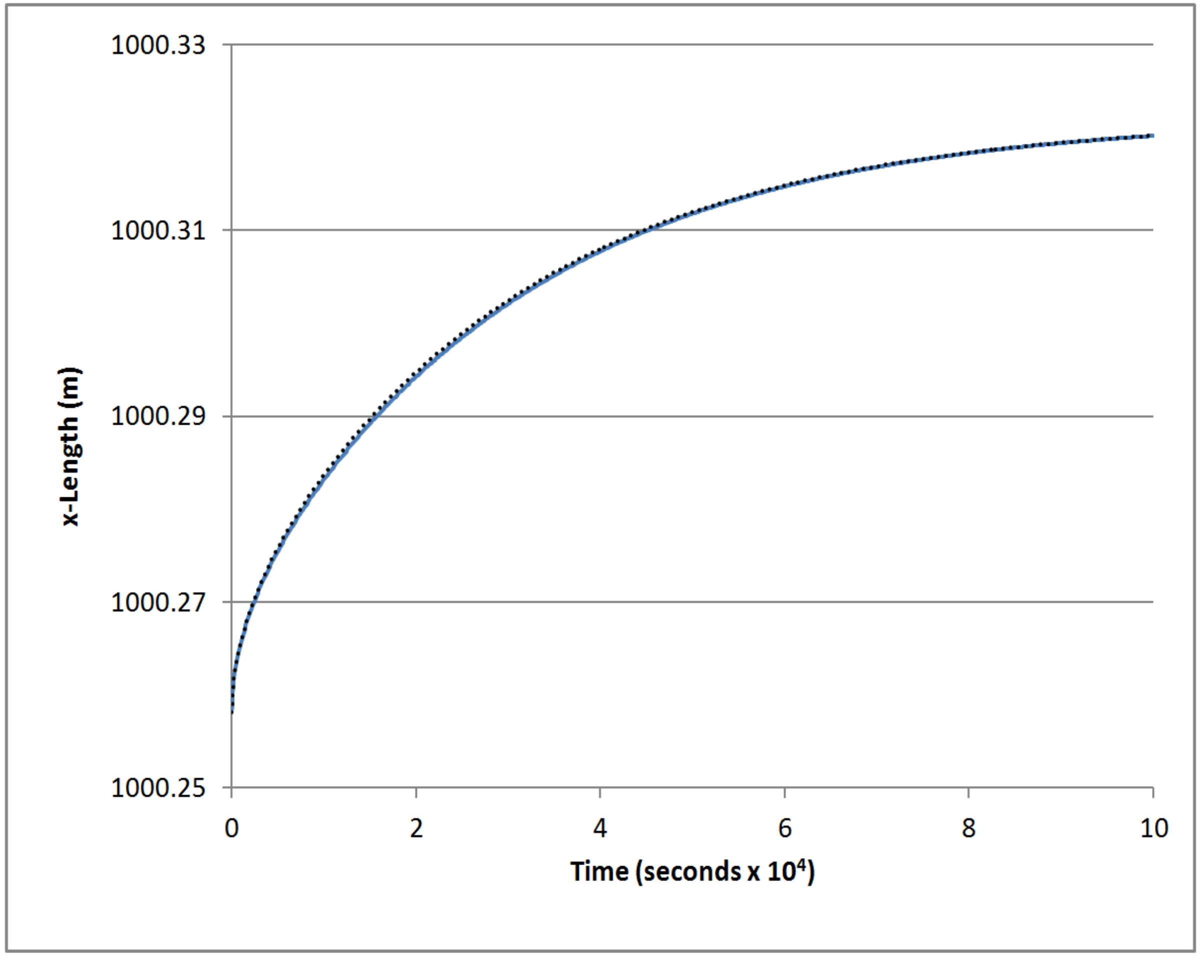
Mandel-Cryer Effect

- Abousleiman *et al.* (1996) analytical solution
- Fluid-filled porous medium, 2D geometry
- Compress medium at top and bottom; drainage occurs laterally
- Center pore pressure reaches a maximum and then declines

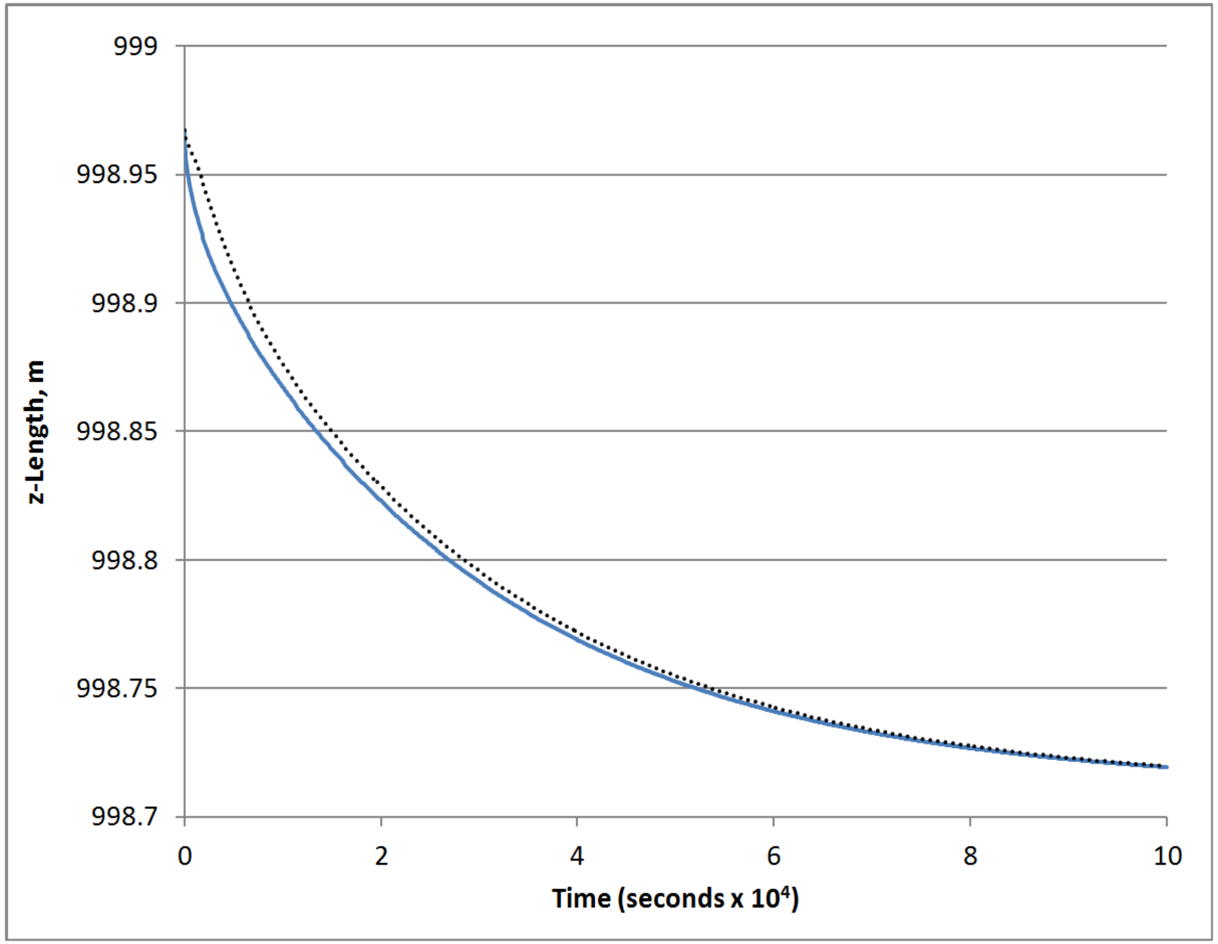
Center Pore Pressure Match



X-direction Length Match



Z-direction Length Match



Stress Tensor Calculation

- Uniform grid
- Injection source at center
- Constant rock properties
- Constant injection rate
- Single phase
- Constant stress on boundaries

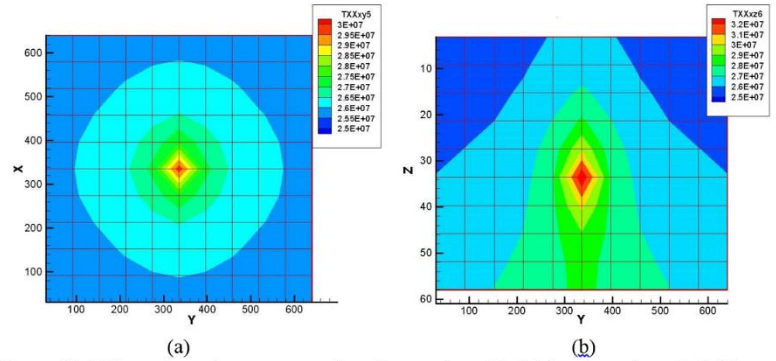


Figure 4.2.5. Normal xx-stress cross sections for xy-plane, K=5 (a) and xz-plane, J=6 (b) after three years of injection.

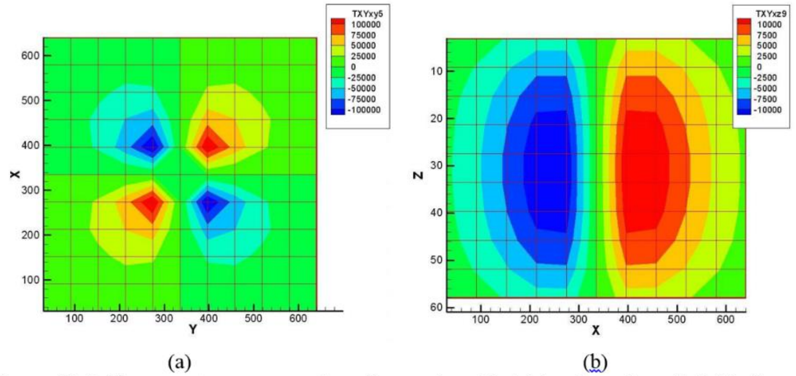


Figure 4.2.6. Shear xy-stress cross sections for xy-plane, K=5 (a) and xz-plane, J=9 (b) after three years of injection.

Example rz Problem

- Yamamoto et al. (2013)
- 100 m aquifer, 1000 m caprock above, 500 m below
- Outer radius of 4100 m
- Equilibrium stress and pressure fields initially
- Mohr-Coulomb failure in upper caprock
- 50 kg/sec CO_2 injected into aquifer at center, 500 days

Simulation Results

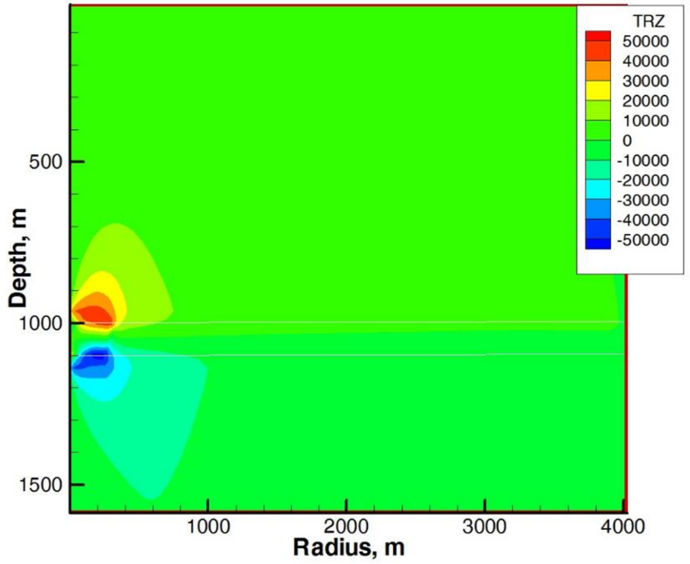


Figure 4.2. Shear stress rz-component after 500 days injection.

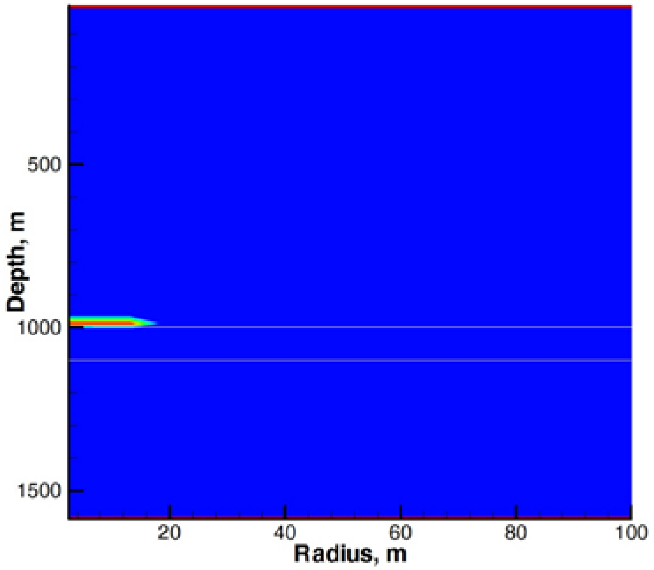


Figure 4.3. Region of caprock failure, just above the aquifer

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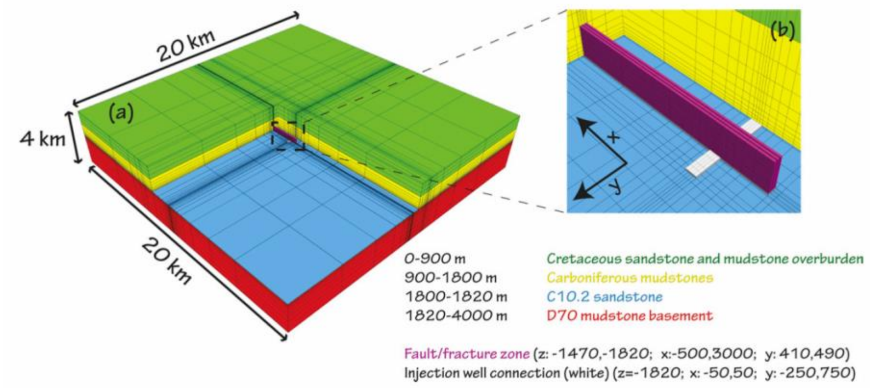
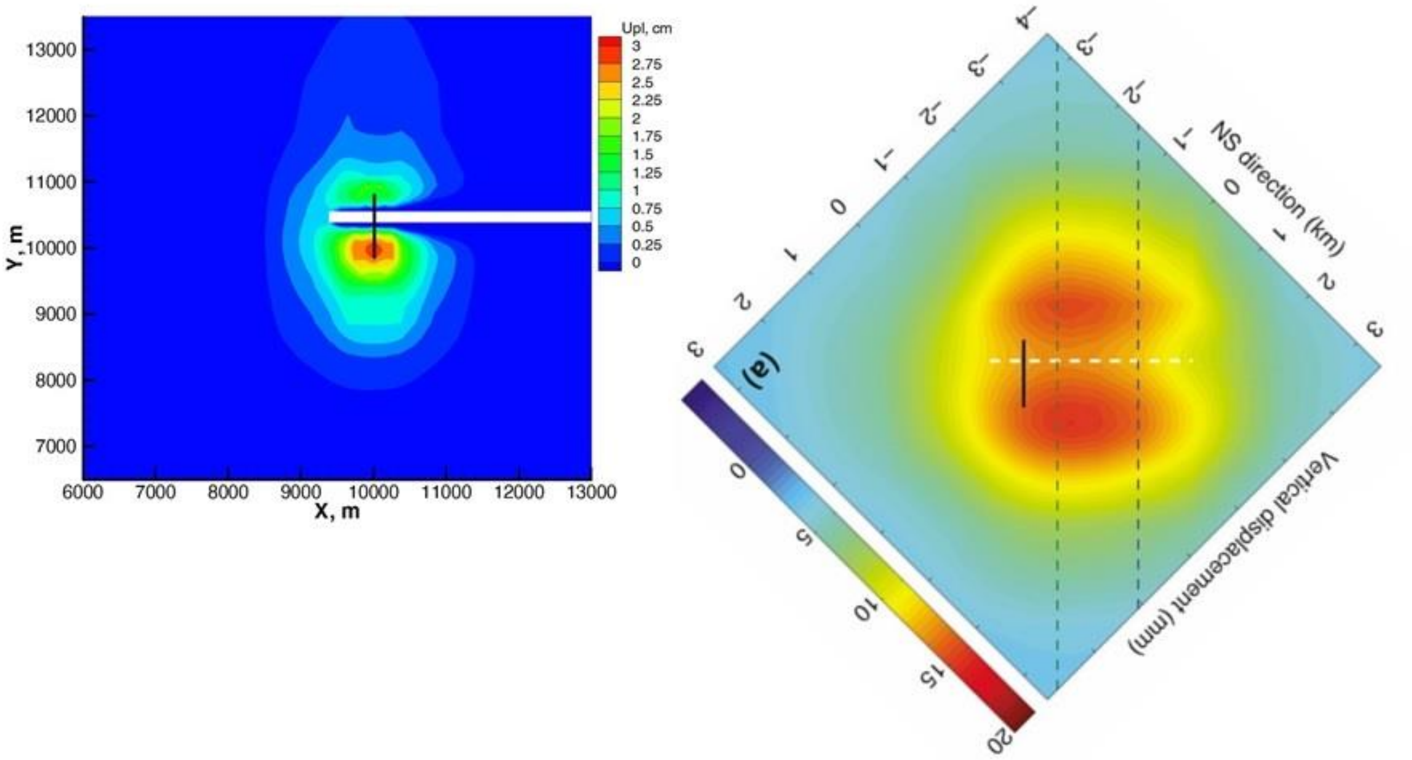
Rinaldi and Rutqvist (2013)

- In Salah well KB-502 double-lobe uplift pattern
- Measured using Interferometric Satellite Aperture Radar (InSAR)
- Explained from presence of a deep vertical fracture



- Four geologic layers, plus sublayers; 1 km horizontal injection well; 80 m wide vertical fracture
- Time-dependent permeability for fracture and aquifer layer to match observed pressure data
- Anisotropic geomechanical properties (fracture) approximated as isotropic in TOUGH2-CSM

Uplift Comparison



Surface uplift for Rinaldi and Rutqvist (2013) (right) and TOUGH2-CSM (left). Solid black lines are wells and white lines are fracture.

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Concluding Remarks

Significant effort and progress have been made at CSM to develop TOUGH2-CSM, an advanced reservoir simulator

- Developed a three-phase flow module (K. Pruess)
- Coupling pressure and temperature effect on rock mechanical deformation for multiphase flow
- Integrating geochemical reactions, being developed
- Improving parallel computing technologies
- Developing fracture conceptual models

We are looking for collaboration for further model improvement and application and welcome CCSU communities to review and use the code!

Concluding Remarks (2)

- The world in the last decade has seen significant enthusiasms and activities in CO2 sequestration. However, the trends will go slow down, because primarily of the economical factor
- The best options for carbon management currently or in the near future:
  - EOR in mature oil/gas reservoirs
  - EOR/EGR in unconventional shale gas/oil formations
- Modeling tools and reservoir simulation will play a critical role in assessing long-term performance of CO_2 GS system from engineering design to long-term monitoring, because of the large time and spatial scales involved with CO_2 geological storage.

Acknowledgement

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- **US DOE (NETL)**

Thanks!

Questions?

Thanks!