Chemical Reaction Modeling with Application to CO_2 Storage in Ultramafic Rocks

Sara F. Farshidi,
Lou Durlofsky, Hamdi Tchelepi

SCCS Annual Meeting
May 27-28, 2015

Outline

- Reactive transport modeling in AD-GPRS
- Ultramafic rocks
- Modeling a natural weathering system
- CO_2 sequestration in ultramafic rocks
- Future work

AD-GPRS

- Advanced research simulator
- Framework for exploring new simulation techniques
- Research tool for optimization studies

- Generalized multi-phase black oil / compositional / thermal model
  - Flexible variable set / implicitness
  - Unstructured grids/MPFA
  - Advanced linear/non-linear solvers
  - Multi-segment well model
  - Chemical reaction modeling
  - Geomechanics coupling

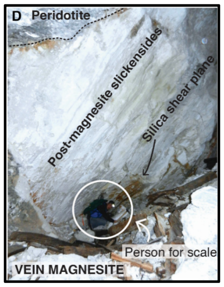
Reservoir Engineering Simulators

- Advanced multiphase flow treatment
  - Capillarity/Hysteresis
  - Phase disappearance/reappearance
- Advanced EOS

- AD-GPRS, chemical reaction development:
  - Element-based reactive transport
  - Natural variable formulation
  - Deposition modeling
  - Overall-composition variable formulation
  - Applied to: In-situ upgrading of oil-shale, CO_2 sequestration in saline aquifers
  - Application to CO_2 sequestration in ultramafic rocks

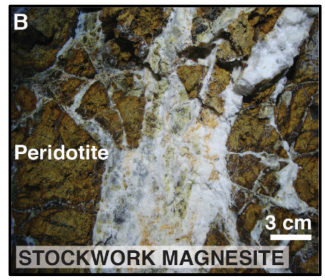
Ultramafic Rocks

- Mantle rock, tectonically exposed
- Mafic minerals: rich in magnesium and iron
- Ultramafic rocks: composed of more than 90% mafic minerals; e.g., peridotites
- Peridotites containing forsterite (Mg_2SiO_4) considered here



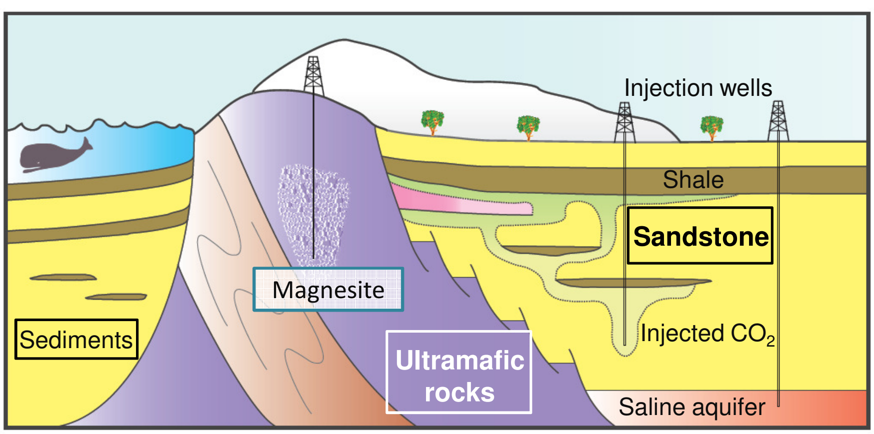
$Mg_2Si_2O_4 + 2CO_2 \leftrightarrow 2MgCO_3 + 2SiO_2$

Forsterite		Magnesite
1 kg	0.6 kg	1.6 kg



From: Pablo Garcia del Real, Stanford University

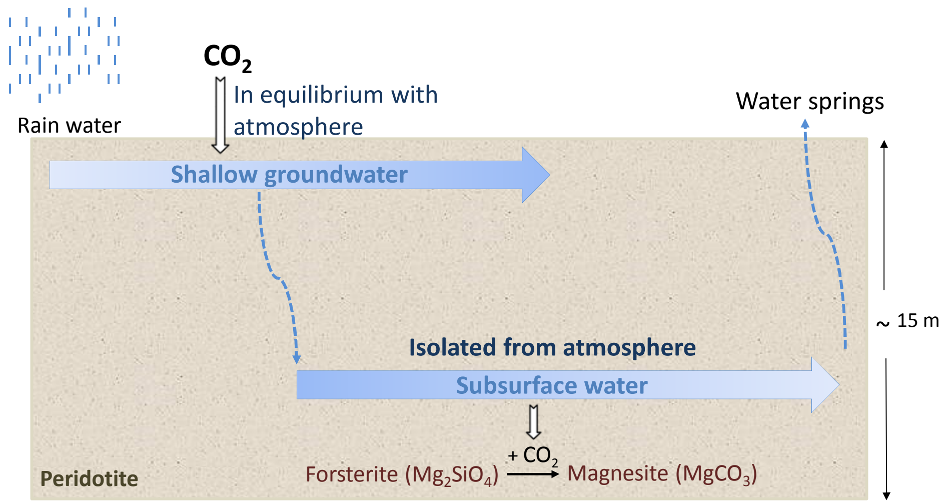
Carbon Storage in Ultramafic Rocks



From: Pablo Garcia del Real, Stanford University

Natural Peridotite System

- Oman Ophiolite Peridotite: natural analog; low temperature weathering system sequesters $10^4 – 10^5$ tons CO_2 annually



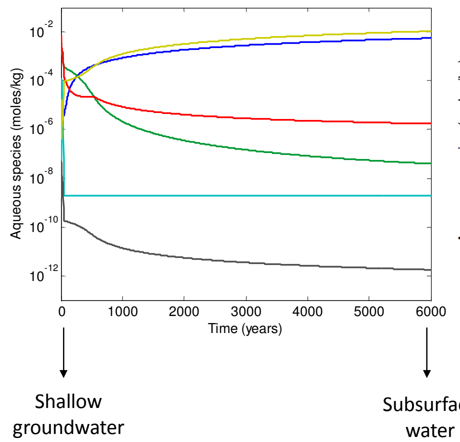
Reaction Path Modeling: Subsurface Water

- 23 species: 13 aqueous species and 10 minerals
- 8 elements
- 5 equilibrium and 10 kinetic reactions
- Modeled as batch reactions: single grid block

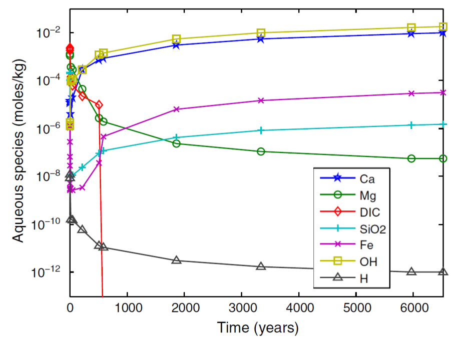
- 3 primary minerals: forsterite, enstatite, diopside
- 6 secondary minerals: chrysotile, calcite, dolomite, magnesite, brucite, quartz
- Halite

Reaction Path Modeling: Subsurface Water

This study

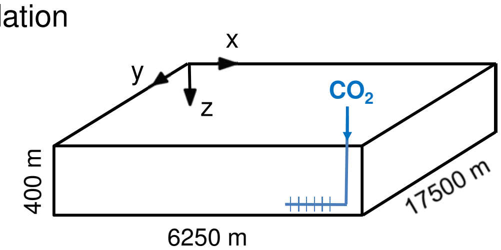


Paukert et al., 2012



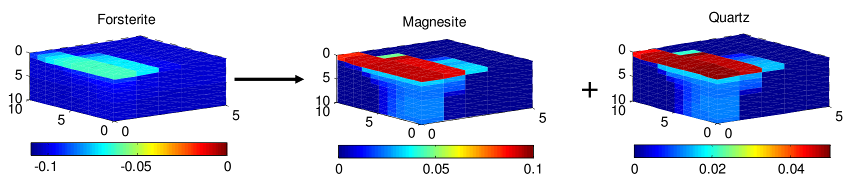
CO_2 Sequestration Case Study

- Permeability: 10 md, porosity: 1%
- Reservoir conditions: 200 bar, 90º C
- 1 MT/year CO_2 injected for 40 years; overall 4% of pore volume
- 10×5×10 grid blocks
- Modeling porosity and permeability changes
- Natural variable formulation



Mineralization Results through Time

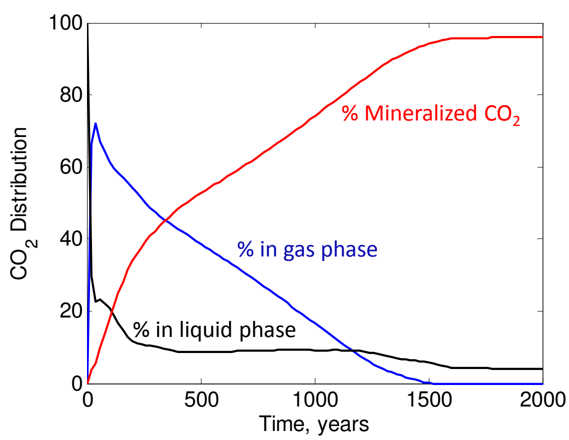
2000 years



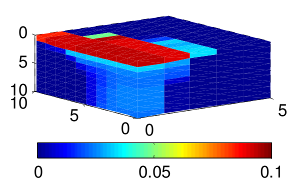
$2CO_2$ + $Mg_2Si_2O_4$ → $2MgCO_3$ + $2SiO_2$

- All plots are in units of kmol/m^3 bulk volume

Mineralization through Time

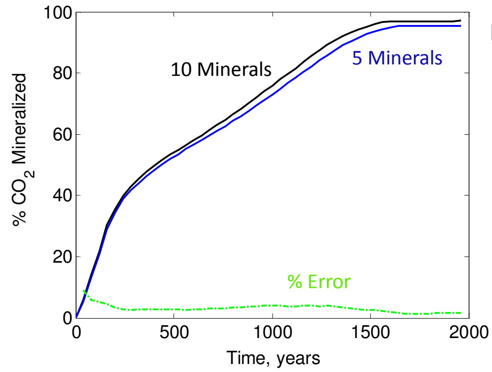


Magnesite profile at 2000 years (kmol/m^3 bulk volume)



10 Minerals versus 5 Minerals

- System of reactions can be modified to include only 5 minerals as the other minerals have minimal effect
- Larger time steps possible
- Model runs 50 times faster



New set of reactions includes:

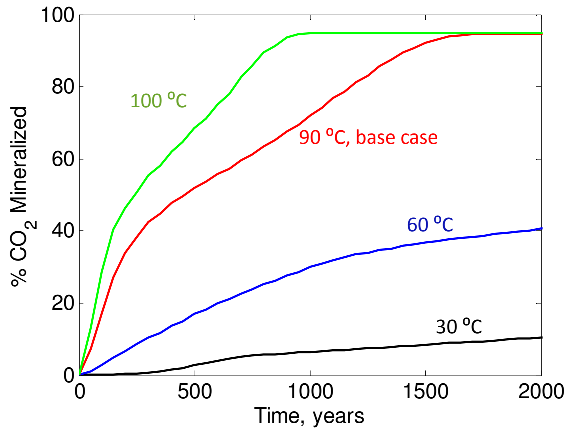
- 17 species: 12 aqueous, 5 minerals
- 7 elements
- 5 equilibrium and 5 kinetic reactions
- 1 primary mineral: forsterite
- 4 secondary minerals: chrysotile, magnesite, brucite, quartz

Sensitivity Studies

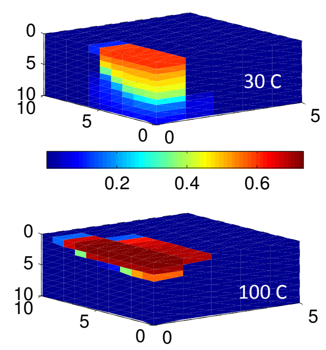
- Temperature dependence
- Pressure dependence
- Effect of permeability
- Effect of porosity
- Vertical grid refinement
- Well management: brine recycling

Temperature Dependence

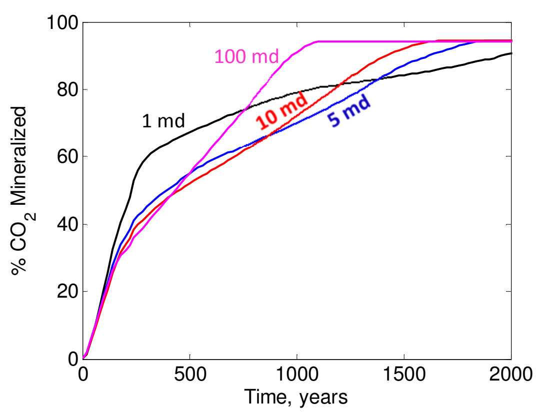
- As temperature increases:
  - Faster kinetics
  - Larger plume



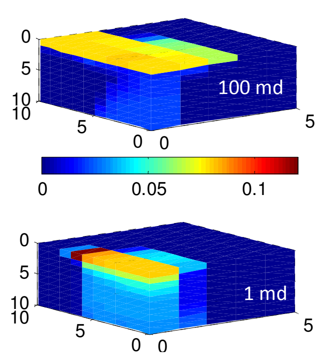
Gas saturation at 100 years



Permeability Dependence



Magnesite at 2000 years
(kmol/m^3 bulk volume)



Conclusions

- Implemented reaction modeling in AD-GPRS using both natural and overall-composition variable formulations
- Examined reaction pathways for CO_2 mineralization in ultramafic rocks (previously considered sandstones)
- Performed 3D reactive transport modeling for CO_2 storage in ultramafic rocks; more than 90% mineralization in many cases
- Plume shape is crucial in accelerating kinetics at large scales
- Temperature is a key factor in both kinetics and plume shape
- Well management strategies can be used to accelerate mineralization

Future Work

- Model realistic fractured systems
- Consider non-isothermal scenarios; e.g., co-injecting hot water
- Represent effects of geochemistry on formation properties in more detail
- Incorporate geomechanical effects to simulate chemically-induced fractures

Acknowledgements

- Pablo Garcia del Real, Geological Sciences, Stanford University
- Denis Voskov
- Kate Maher, Geological Sciences, Stanford University

Questions?