Chemical Reaction Modeling with Application to CO\(_2\) Storage in Ultramafic Rocks

Sara F. Farshidi, Lou Durlofsky, Hamdi Tchelepi

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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, CO₂ sequestration in saline aquifers
  - Application to CO₂ 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 (\(\text{Mg}_2\text{SiO}_4\)) considered here

\[
\text{Mg}_2\text{Si}_2\text{O}_4 + 2\text{CO}_2 \leftrightarrow 2\text{MgCO}_3 + 2\text{SiO}_2
\]

<table>
<thead>
<tr>
<th>Forsterite</th>
<th>Magnesite</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 kg</td>
<td>0.6 kg</td>
</tr>
</tbody>
</table>

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

$\text{CO}_2$ in equilibrium with atmosphere

Rain water

Water springs

Shallow groundwater

Isolated from atmosphere

Subsurface water

Forsterite (Mg$_2$SiO$_4$) $+ \text{CO}_2$ Magnesite (MgCO$_3$)

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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

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Reaction Path Modeling: Subsurface Water

This study

Paukert et al., 2012

CO₂ Sequestration Case Study

- Permeability: 10 md, porosity: 1%
- Reservoir conditions: 200 bar, 90° C
- 1 MT/year CO₂ 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

2\text{CO}_2 + \text{Mg}_2\text{Si}_2\text{O}_4 \rightarrow 2\text{MgCO}_3 + 2\text{SiO}_2

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

Mineralization through Time

% Mineralization CO$_2$

% in gas phase

% in liquid phase

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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

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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

![Graph showing temperature dependence with curves for 30°C, 60°C, 90°C, and 100°C, with 100°C as the base case.]

Permeability Dependence

![Graph showing permeability dependence with curves for 1 md, 5 md, 10 md, and 100 md, with 100 md as the base case.]

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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
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Questions?