Reactive Transport Models with Geomechanics to Mitigate Risks of CO2 Utilization and Storage
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PI-Milind Deo, University of Utah
Idaho National Laboratory

Presenter: Hai Huang, Energy Resource Recovery & Sustainability
Idaho National Laboratory
Large scale injection of $\text{CO}_2$
Mechanisms: trapping, dissolution, carbonation
Is safe storage of large amounts of $\text{CO}_2$ feasible?
Risks
  – Overpressure
  – Leaks
  – Mechanical integrity of the seals
  – Induced seismicity
Extensive work and publications on each and every aspect

Integrated, physics-based, geochemical and geomechanical model capable of predicting fracturing and slipping of natural fractures
Problem: Non-availability of CO2 Reactive Transport Model with Physics Based Geomechanics

Approach: Couple ARTS and DEM and Validate

Better prediction of mechanical changes due to CO2 transport and reactions

Outcomes:
- Induced Seismicity Prediction
- Injectivity loss or gain, overpressure, fault or fracture leakage

Tools Currently Available:
- ARTS: Advanced Reactive Transport Simulator at the University of Utah
- DEM: Discrete Element Method
- CT: Computer Tomography

Validation tools:
- High-pressure Core Flooding and Micro-CT Visualization

Tools at the Idaho National Laboratory:
- DEM based Geomechanics
Project Scope

• Experimental study for model validations
  – Corefloods
    • Three possible mineralogies, sa
    • Characterization using XRD, ICP-MS
  – High-resolution micro computed tomography

• Modeling
  – Multiphase reactive transport simulator – ARTS
  – Discrete-element model (DEM) for geomechanics from INL
  – Different coupling schemes: fully coupled vs. sequential coupling
Experiments on Reactions

Core Pressure: 2,000 psi
Confining Pressure: 3,000 psi
Reaction temperature: 60 °C
Cores (7”): Sandstone, Limestone, and Dolomite
CO₂ : Brine: 1.41 ml/min : 1 ml/min
Micro-CT Imaging
## Batch Results – ICP MS

All concentrations in mg/Kg

<table>
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<th></th>
<th>Na</th>
<th>Mg</th>
<th>Si</th>
<th>Cl</th>
<th>K</th>
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<td>Dolomite</td>
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<td>182.5</td>
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<td>1233</td>
<td>10</td>
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Limestone and dolomite show dissolution
Experimental Conclusions

- Significant visible dissolution with increased porosities in limestone and dolomite
- Lesser dissolution in sandstone – still visible in micro-CT
- ICP-MS results confirm the dissolution findings
- XRD values before and after do not show significant changes
Multiscale Reactive Transport Modeling and High-Performance Computing

- Pore-scale reactive transport models developed at INL
  - Level set; Phase field; Smoothed particle hydrodynamics
- Advanced reactive transport simulator (ARTS)
  - Fully coupled, fully implicit approach
  - Massively parallel; Adaptive mesh refinement (AMR)
Pore-scale Reactive Transport Modeling

Permeability-porosity evolution due to mineral precipitation/dissolution under different transport and reaction regimes

- **Diffusion dominated transport & slow reaction**
  - $Pe=0.086$, $Da=0.001$

- **Diffusion dominated transport & fast reaction**
  - $Pe=0.086$, $Da=0.1$

- **Advection dominated transport & fast reaction**
  - $Pe=8.6$, $Da=0.1$

![Graph showing $K/K_0$ vs $\varepsilon/\varepsilon_0$ for different parameter values]
A Geochemical Simulator For Complex Geometries (DFN)

- A fully implicit non-isothermal geochemistry compositional simulator
- Unstructured mesh
- Different discretization and fracture representation methods
- Verification and validation
- Applications and parallelization performance evaluation
Coupled DFN-Porous Matrix Results

–The fracture/fault effect: fracture network case

Free and dissolved CO₂ distribution at 100 days with or without fracture network

Almost all free CO₂ accumulates at the top due to channeling through fractures.

Free CO₂ distribution with or without fracture network

Dissolved CO₂ distribution with or without fracture network
Numerical Modeling of Coupled Processes

- **Loose Coupling / Operator Split**
  1. Solve PDE1
  2. Pass Data
  3. Solve PDE2
  4. Move To Next Timestep

- **Sequential Coupling w/Iteration**
  1. Solve PDE1
  2. Pass Data
  3. Solve PDE2
  4. Pass Data
  5. Return to 1 Until Convergence
  6. Move To Next Timestep

- **Fully Coupled**
  1. Solve PDE1 and PDE2 simultaneously in _one_ system
  2. Move To Next Timestep
Jacobian-free Newton Krylov (JFNK) Solution For Nonlinear Coupled THMC Processes

- Newton’s method is used to solve the nonlinear system
  \[ F(u) = 0, \text{ or } F(u^{n+1}) < \text{tol} \]

- The resulting linear system and nonlinear iteration are
  \[ J\delta u^{n+1} = -F(u^n) = 0, \quad u^{n+1} = u^n + \delta u^{n+1} \]

- Using a Krylov method (GMRES) to solve the linear system only requires a matrix-vector product (the Jacobian never appears alone)
  \[ \delta u^{n+1,k} = a_0 r_0 + a_1 J r_0 + a_2 J^2 r_0 + \ldots + a_k J^k r_0 \]

- This matrix-vector product (for generic \( \mathbf{v} \)) may be approximated by
  \[ J\mathbf{v} \approx \frac{F(u + \epsilon \mathbf{v}) - F(u)}{\epsilon} \]
Challenges for Simulating Geomechanical Response Due to Injection

Fracturing coupled with flow:
- Initiation & propagation of new cracks during injection
- Interactions between hydraulic fractures and natural existing fractures
- Permeability changes of fractures as fluid pressure and temperature change

Conventional continuum thermoporoelastic models are inadequate:
- Empirical laws to trigger failure
- Empirical laws for post-failure mechanics: sliding, dilation etc.

Need more “physics” based models for more robust modeling:
- Fracture propagations,
- Reactivation of pre-existing fractures and permeability evolutions
Discrete Element Model (DEM) for Fracturing and Geomechanics Under Stimulations

DEM Model Framework

- Represent material, including heterogeneity and anisotropy, by a network of mechanical elements connected by springs or beams, elastic or viscoelastic, etc.
- Impose boundary conditions (stress, strain)

Force and Moment Balance

\[ \vec{F}_{i,j} = k_n (d_{i,j} - d_{i,j}^0) + k_s \frac{1}{2} (\phi_{i,j} + \phi_{j,i}) \hat{s}_{i,j} \]

\[ \vec{M}_{i,j} = k_s \mathcal{A} \left[ \frac{\Phi}{12} (\phi_{i,j} - \phi_{j,i}) + \frac{1}{2} \left( \frac{2}{3} \phi_{i,j} + \frac{1}{3} \phi_{j,i} \right) \right] \]
Simulations of multistage hydraulic fracturing
Multistage hydraulic fracturing at high injection rate
Mutlistage hydraulic fracturing at high injection rate

Stress fields

Wellbore pressure
Multistage hydraulic fracturing at high injection rate

Fracture path

Fluid pressure
Mutlistage hydraulic fracturing at high injection rate
Effects of injection rates

Q

2Q
Reactivation of natural fractures

1. Injection rate: 2.5Kg/s
2. Initial fluid pressure: 20MPa
3. Max. injection pressure: 55MPa
4. No leakage from fracture to matrix is considered
5. Only opening and slip of existing cracks are considered
Reactivation of natural fractures
Reactivation of Natural Fractures: slipping vs. opening
Accomplishments to date

• Developed apparatus for batch and core flooding experiments under elevated temperature and pressure
• Conducted batch experiments for reaction kinetics
• Applied pore-scale models for porosity-permeability constitutive relationships for relevant rocks.
• Implemented the porosity-permeability relationships into the continuum reactive transport simulator
• Coupled 2D DEM model with flow simulator under two extremes:
  – Hydraulic fracturing
  – Reactivation of pre-existing fractures
Summary

• Key findings:
  – Mineral dissolution and precipitation strongly affects permeability of fractured reservoir
  – Fracturing and geomechanics response are important to wellbore injectivity

• Future plan
  – Core flooding experiments, chemical analysis and core imaging
  – Validate pore-scale and continuum reactive transport models with experiments
  – Coupling 3D DEM with flow simulator
• Backup slides
Batch Experimental System

Oven 60°C

PG
CO₂
2% NaCl
Limestone
PG
CO₂
2% NaCl
Sandstone
PG
CO₂
2% NaCl
Dolomite
Experimental System
Additional Results

- Dissolution with limestone
- Dissolution and reprecipitation with peridotite
- Effect of gas chemistry
  - Presence of SO₂ in CO₂ causes continuous dissolution of carbonate.
    Anhydrite formation detected
- Implications on injectivity and pressurization
Review of Core Floods

• Generally increased porosity in calcitic/dolomitic systems near injection points

• Carbonation and decreased porosity at the end of the sample over time
DEM Parameter Calibration Using Uniaxial Compression and Tension Tests

Relationships developed between DEM bond parameters and bulk mechanical properties:
- Young’s modulus (E)
- Poisson’s ratio (ν)
- Tensile strength (S_t)
- Compressive strength (S_c)

Simulated nucleation, propagation and growth of microfractures and the final macroscopic failure of rock sample
Model Validation: DEM vs. FEM

Model Parameters
Unconfined boundaries
$T_{heater} = 1000 \, ^\circ F$
$E = 1.0 \times 10^6 \, \text{psi}$
$V = 0.23$
$\alpha = 2.36 \times 10^{-5} \, ^\circ F^{-1}$
$D = 0.55 \, \text{ft}^2/\text{day}$
$t = 40 \, \text{hours}$

Satisfactory match between DEM and FEM in linear elastic regime