Studies for Modeling CO₂ Processes: Pressure Management, Basin-Scale Models, Model Comparison, and Stochastic Inversion

ESD09-056

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Lawrence Berkeley National Laboratory

U.S. Department of Energy
National Energy Technology Laboratory
Carbon Storage R&D Project Review Meeting
Developing the Technologies and Infrastructure for CCS
August 20-22, 2013
Presentation Outline

• Benefit to the Program

• Project Overview and Technical Status
  – Task 1: Optimization of Brine Extraction for Pressure Management and Mitigation
  – Task 2: Basin-scale Simulation of CO$_2$ Storage in the Northern Plains – Prairie Basal Aquifer
  – Task 3: Sim-SEQ Model Comparison
  – Task 4: Efficient Methods for Stochastic Inversion of Uncertain Data Sets

• Accomplishments to Date

• Project Summary
Benefit to the Program

• Task 1 provides technology that improves reservoir storage efficiency while ensuring containment
  – This task develops optimization methods, and associated simulation tools, to design pressure management solutions at minimal cost

• Tasks 2 and 3 provide methodology that supports industries’ ability to predict (or control) CO₂ storage capacity in geologic formations to within ±30 percent
  – Task 2 applies simulation capabilities to evaluate dynamic storage capacity for one of the largest storage reservoirs in North America
  – Task 3 conducts model comparison for a selected GCS site to better understand and quantify model uncertainty

• Task 4 develops technology to ensure 99% storage permanence
  – This task provides new methods to substantially improve current inversion capabilities for site characterization and monitoring data
Project Overview Task 1:
Optimization of Brine Extraction for Pressure Management and Mitigation

- **Objectives**
  - Develop optimization methodology for pressure management via brine extraction
  - Conduct pressure management with minimal brine extraction volumes while meeting desired reservoir performance goals

- **Impact-Driven Pressure Management (IDPM)**
  - Define specific (local) performance criteria (e.g., maximum pressure near fault zone, maximum leakage rate, maximum caprock pressure)
  - Via smart search algorithms, automatically optimize well locations and brine extraction rates to meet performance criteria

Example: Critically stressed fault
Technical Status Task 1:
Optimization of Brine Extraction for Pressure Management and Mitigation

- **Optimization Methodology Development (FY12 and FY13)**
  - Develop inverse modeling and optimization methodology using iTOUGH2 coupled to analytical solution for simplified studies (in Birkholzer et al., IJGGC, 2012)
  - Incorporate higher-fidelity simulators such as multiphase flow models into optimization framework for complex applications
  - Improve optimization efficiency for well placement scenarios coupling global and gradient-based methods

- **Pressure Management Applications (FY12 and FY13)**
  - Proof-of-concept studies (e.g., simplified geology and scenarios, single and multiple performance criteria, active and passive relief) (in Birkholzer et al., IJGGC, 2012)
  - More realistic scenarios involving multiphase inversions to handle more complexity (e.g., complex geology, heterogeneity, CO₂ breakthrough)
  - IDPM optimization of one real CO₂ sequestration site

- **Expansion of Optimization Method to Storage Management (FY14)**
  - Design and demonstrate storage management optimization for improved injectivity and enhanced CO₂ trapping
  - Design of real-time storage management schemes
Task 1:
Optimization Methodology Using iTough2 and Suite of Forward Simulation Tools

- iTough2 provides inverse modeling capabilities for multi-phase simulator TOUGH2 or, via PEST interface, other forward prediction tools
- For IDPM, iTough2 was expanded to include new global search algorithms, and was linked to efficient vertical-equilibrium forward simulators

Forward Predictors

1. Analytical Solution
   - Single-phase flow in homogeneous infinite multi-layer systems
   - No CO₂ migration

2. Simulators Based on Vertical Integration
   - Sharp-Interface Models
   - Vertically Integrated Multi-Phase Models
   - CO₂ migration in complex and heterogeneous systems

3. Simulator TOUGH2
   - Multi-phase flow in full 3D systems
Task 1: Efficient Optimization Strategies for Large-Scale Pressure Management Problems

- Specifically for well placement problems, objective functions can have multiple local optima in the solution space; in such cases, global optimization methods are preferred (but they are not as efficient because they multiple forward runs).
- Gradient-based local optimization methods are faster and better suited for optimization of extraction/injection rates.
Task 1: Two-Step Strategy for Optimization of Well Placement and Brine Extraction

- Efficient solution is achieved by combining a global parallel search algorithm for well placement with a gradient-based local search algorithm for estimation of extraction rates.
- Time-dependent extraction rates are defined as functional relationships (so that a few functional parameters need to be inverted for, rather than stepwise rates).

**Differential Evolution Algorithm (DEA)**
- Optimize well locations with simplified models and reduced number of parameters (e.g. fixed extraction rates).
- Wells constrained to be at sufficient distance away from CO₂ plume.

**Levenberg-Marquardt Algorithm, (LM)**
- Use LM to estimate optimum time-dependent actual extraction rates satisfying performance criteria.

**Main Stages of Differential Evolution Algorithm (Storn and Price, 1997)**
- Initialization
- Mutation
- Crossover
- Selection
Task 1: Verification of Solution Accuracy and Efficiency

**Test Problem 1:** Verification against a problem with known solution. Two-step method reached the correct solution.

**Test Problem 2:** A scenario with heterogeneity and multiple injection wells near a fault. DEA and LM are used sequentially to optimize well placement, injection rates, and extraction rates for preventing fracturing and fault reactivation.
Task 1:
Application of IDPM for CO$_2$ Injection in the Vedder Formation (Southern Joaquin Valley, California)
Task 1:
Results for Injection of 5 Mt CO₂ per year Over 50 Years Without Pressure Management

Homogeneous Reservoir (Time=50yr, $k_{\text{reserv}}/k_{\text{fault}}=100$)

Heterogeneous Reservoir (Time=50yr, $k_{\text{reserv}}/k_{\text{fault}}=100$)
Task 1:
Optimized Well Placement and Extraction Rates for Homogeneous Scenario
Task 1:
Optimized Well Placement and Extraction Rates for Heterogeneous Scenario
Project Overview Task 2:
Basin-scale Simulation of CO₂ Storage in the Northern Plains – Prairie Basal Aquifer

- **Objective**
  - Conduct high-performance regional-scale simulations of future CO₂ storage scenarios in the Northern Plains – Prairie Basal Aquifer (Alberta and Williston Basin)
    - determine the distribution, migration, and long term fate of multiple CO₂ plumes
    - evaluate pressure perturbation and brine migration effects
    - evaluate the dynamic storage capacity of the aquifer

- **Technical Status**
  - Obtained 3D geologic model developed based on characterization data from our project partners EERC (United States) and AITF (Canada)
  - Analyzed spatial variability of rock properties and in situ reservoir conditions, and determined potential storage sites and injectors
  - Developed 3D CO₂-brine flow model with local mesh refinement around 127 injection wells at 16 storage sites over a 1500 km x 1600 km domain
  - Predicted the system response to multiple CO₂ injections; comparison with simpler solutions is ongoing
Task 2:
3D Geologic Model for the Basal Aquifer

- EERC/AITF collected all well data in the Alberta Basin and the Williston Basin covering the model domain
- The Basal Aquifer consists of 25 model layers
- Porosity/permeability in all layers was generated using geostatistical approach with conditioning
Project Overview Task 3: Sim-SEQ Model Comparison

**Objective**
- Sim-SEQ intends to understand and quantify uncertainties arising from conceptual choices made in model development.
- Ultimate goal is to demonstrate that the system behavior of GCS sites can be predicted with confidence and that subsurface processes expected in response to CO₂ storage are sufficiently well understood.

**Technical Status**
- Sim-SEQ currently involves 16 modeling teams from 8 countries.
- Modelers are at present focusing on one selected GCS field site, i.e., the S-3 site, patterned after the Phase III CO₂ injection project at Cranfield, MS.
- Predictive flow models have been developed and model-to-model comparison has been finalized.
- Model refinement using field observations and model-to-data comparison ongoing.

![Location map of the S-3 site including the Detailed Area Study (DAS); Courtesy of JP Nicot](image)
Task 3:
Sample Results from Model-to-Model Comparison

F1: ~70 m
F2: ~30 m
F3:

Acknowledgment: JP Nicot (BEG)
Task 3: Interpretation Based on Statistical Analysis

<table>
<thead>
<tr>
<th>Factors</th>
<th>F-2 Breakthrough Time, day</th>
<th>F-3 Breakthrough Time, day</th>
<th>Max Pressure 30d, MPa</th>
<th>Max Pressure 180d, MPa</th>
<th>Max Pressure 365d, MPa</th>
<th>RMSE bpw2, MPa</th>
<th>RMSE bpw3, MPa</th>
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- Modeling scheme plays the most significant role
- Response variables are more sensitive to input parameters at intermediate times
- Simplified models (homogeneous and isotropic) produce the largest deviances
- Highly complex models (3-D heterogeneous and anisotropic) models have more simulation errors compared to models with intermediate levels of complexities
- Model prediction could be improved with more site-specific parameters/factors
- Model refinement using observation data will likely reduce the range of predictions
Project Overview Task 4: Efficient Methods for Stochastic Inversion of Uncertain Data Sets

• Objective
  – Develop stochastic inversion methods as a superior calibration method for joint analysis of multiple types of uncertain and often very large data sets
  – Improve computational efficiency of existing inversion methods
  – Alleviate the computational hurdles associated with heterogeneity characterization and plume monitoring in field-scale CO₂ applications

• Technical Status
  – Introduced Krylov subspace methods to solve the geostatistical inversion system and designed efficient preconditioners
    o Avoids direct computing and storage of the sensitivity matrix
    o Significantly reduces the memory requirement from hundreds of GBs to a few GBs for large 3-D problems
  – Introduced model reduction methods to reduce the size of the forward model
    o Designed geostatistical reduced-order models (GROMs) for inverse problems with a large number of unknowns and a limited number of measurements
    o Reduced the size of the forward model by orders of magnitude
Task 4:
Sample Results for Stochastic Inversion using GROM

- Left column shows synthetic example with true random $\ln(K)$ field (top), estimated field using GROM (middle), and estimated field with full model.
- Graph below left shows correlation between estimated and true hydraulic head.
- Graph below right shows correlation between estimated and measured pressure data.
Accomplishments to Date

• Task 1: Optimization of Brine Extraction
  – Developed efficient optimization method that minimizes brine extraction volumes while meeting defined reservoir management targets
  – Successfully applied optimization method to complex injection scenarios and reservoir conditions

• Task 2: Basin-scale Simulation of CO₂ Storage
  – Developed high-performance model of Northern Plains – Prairie Basal Aquifer and evaluated dynamic storage capacity of this important storage reservoir

• Task 3: Sim-SEQ Model Comparison
  – Built Sim-SEQ into a multi-national model comparison initiative with involvement of 16 international modeling teams
  – Conducted model-to-model comparison and interpretative analysis of model discrepancies

• Task 4: Efficient Methods for Stochastic Inversion
  – Introduced stochastic inversion for joint analysis of multiple types of uncertain data related to GCS projects and significantly improved inversion efficiency
Summary

• Key Findings / Lessons Learned from Modeling Tasks
  – Task 1: Smart and efficient inversion methods are now available for design of optimized pressure management solutions
  – Task 2: High-performance and high-fidelity models allow GCS predictions for very large 1500 km x 1600 km domain
  – Task 3: Model comparison results suggest limited uncertainty with respect to several performance measures
  – Task 4: Stochastic inversion has notable potential for joint analysis of large data sets

• Future Plans
  – Task 1: Expansion of optimization methods to real-time storage management for better pressure control, improved injectivity, and enhanced trapping
  – Task 2: Ending
  – Task 3: Continuation of model-to-data comparison and iterative model improvement
  – Task 4: Application of stochastic inversion methods to data from CO₂ storage sites (e.g., using pumping test and CO₂ injection data from the pilot test at Ketzin, Germany)
Appendix

– These slides will not be discussed during the presentation, but are mandatory
Appendix: Organization Chart

- “Studies for Modeling CO₂ Processes” is a subtask of LBNL’s Consolidated Sequestration Research Program
- “Studies for Modeling CO₂ Processes” has four main tasks with principal investigators identified as PI
  - Task 1: Abdullah Cihan, Marco Bianchi, and Jens Birkholzer (PI)
  - Task 2: Quanlin Zhou (PI) and Dorothee Rebscher
  - Task 3: Sumit Mukhopadhyay (PI) and Jens Birkholzer, and several international modeling teams
  - Task 4: Xiaoyi Liu and Quanlin Zhou (PI)
- List of scientific staff

<table>
<thead>
<tr>
<th>Name</th>
<th>Title</th>
<th>Role in Task/Subtask</th>
</tr>
</thead>
<tbody>
<tr>
<td>Jens Birkholzer</td>
<td>PI and Research Scientist</td>
<td>Lead scientist for Modeling CO₂ Processes</td>
</tr>
<tr>
<td>Abdullah Cihan</td>
<td>Research Scientist</td>
<td>Main scientist working on pressure management</td>
</tr>
<tr>
<td>Marco Bianchi</td>
<td>Postdoctoral researcher</td>
<td>Supporting role in pressure management studies</td>
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<tr>
<td>Barbara Fialeix</td>
<td>Visiting graduate researcher</td>
<td>Supporting role in pressure management studies</td>
</tr>
<tr>
<td>Quanlin Zhou</td>
<td>PI and Research Scientist</td>
<td>Main scientist working on basin-scale simulations</td>
</tr>
<tr>
<td>Dorothee Rebscher</td>
<td>Project Scientist</td>
<td>Supporting role in basin-scale simulations</td>
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<tr>
<td>Sumit Mukhopadhyay</td>
<td>PI and Research Scientist</td>
<td>Main scientist working on Sim-SEQ</td>
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<tr>
<td>Xiaoyi Liu</td>
<td>Postdoctoral researcher</td>
<td>Main scientist working on stochastic inversion</td>
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</table>
## Appendix: Gantt Chart for FY13

<table>
<thead>
<tr>
<th>Task/Milestone</th>
<th>Fiscal Year Quarter</th>
<th>FY13</th>
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<tbody>
<tr>
<td><strong>Task 1: Optimization of Brine Extraction for Pressure Management and Mitigation</strong></td>
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<tr>
<td>Incorporate Higher-Fidelity Simulators into the Optimization Framework</td>
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<td>Test Global Optimization Algorithms</td>
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<tr>
<td>Apply IDPM Methodology to a Realistic Field Site</td>
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<td><strong>Task 2: Basin-scale Simulation of CO₂ Storage in the Northern Plains – Prairie Basal Aquifer</strong></td>
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<td>Assess Dynamic Storage Capacity</td>
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<tr>
<td>Assess Pressure Buildup and Environmental Impact for a Variety of Realistic Scenarios</td>
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<td><strong>Task 3: Sim-SEQ Model Comparison</strong></td>
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<td>Perform Model-to-Model Comparison</td>
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<td><strong>Task 4: Efficient Methods for Stochastic Inversion of Uncertain Data Sets</strong></td>
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<tr>
<td>Develop Stochastic Joint Inversion Methods</td>
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<tr>
<td>Develop Model Reduction Methods for Improved Computational Efficiency</td>
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<td>Methodology Demonstration Using Synthetic Data</td>
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Appendix: Milestone Log for FY13

Task 1: Optimization of Brine Extraction for Pressure Management and Mitigation
- Milestone 4-3 (I), Q2 (3/31/13)
  Title: Develop automated global optimization methods to optimize IDPM options for heterogeneous systems and variable well locations
- Milestone 4-4 (J), Q4 (9/30/13)
  Title: Design and optimize IDPM options for a realistic field site

Task 2: Basin-scale Simulation of CO₂ Storage in the Northern Plains – Prairie Basal Aquifer
- Milestone 4-1 (G), Q2 (3/31/13)
  Title: Apply the developed basin-scale model to assess dynamic storage capacity
- Milestone 4-2 (H), Q4 (9/30/13)
  Title: Apply the developed basin-scale model to a variety of future storage scenarios to assess pressure buildup and environmental impact

Task 3: Sim-SEQ Model Comparison
- No milestone in FY13

Task 4: Efficient Methods for Stochastic Inversion of Uncertain Data Sets
- Milestone 4-6 (L), Q2 (3/31/13)
  Title: Develop stochastic joint inversion methods for pressure/temperature modeling and monitoring
- Milestone 4-7 (M), Q4 (9/30/13)
  Title: Develop model reduction methods and apply joint inversion to a synthetic example


Task 1:
Effects of Critical Pressure and Fault Permeability on ‘Extraction Ratio’

Extraction Ratio: Total Volume of Extracted Brine Divided by Injected CO$_2$