Studies for Modeling CO_2 Processes: Pressure Management, CO_2-EOR Simulation, Model Comparison, and Stochastic Inversion

ESD09-056

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U.S. Department of Energy

National Energy Technology Laboratory
Carbon Storage R&D Project Review Meeting
Developing the Technologies and
Infrastructure for CCS

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Presentation Outline

- Benefit to the Program
- Project Overview and Technical Status
  - Task 1: Pressure Management Optimization Framework

    This task develops optimization methods, and associated simulation tools, to design CO_2 pressure management solutions at minimal cost
  - Task 2: Simulation Capabilities for GCS in Oil Reservoirs

    This task develops rigorous simulation capabilities for modeling GCS in oil reservoirs, with focus on long-term trapping and fate of CO_2
  - Task 3: Sim-SEQ Model Comparison Using Field Data

    This task conducts model comparison for a selected GCS site to better understand and quantify model uncertainty
  - Task 4: Efficient Methods for Stochastic Inversion

    This task provides new methods to substantially improve current inversion capabilities for site characterization and monitoring data
- Accomplishments to Date
- Project Summary

Benefit to the Program

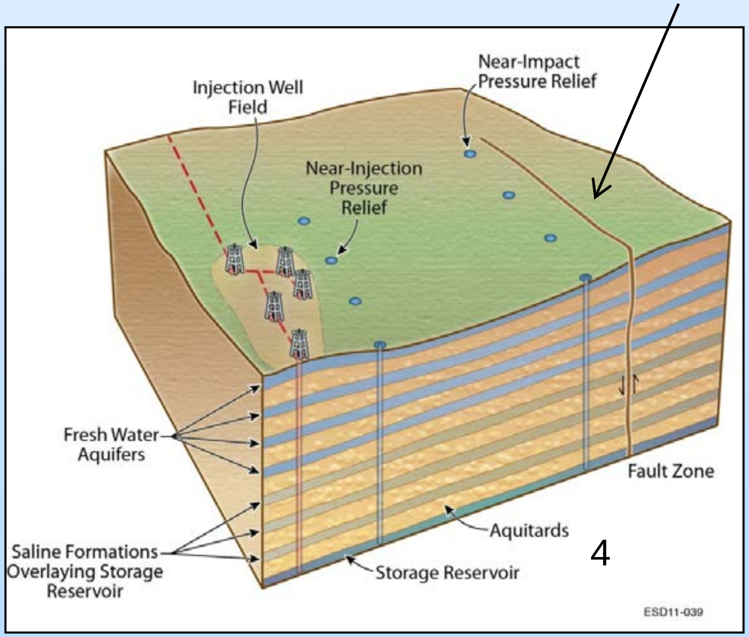
- Task 1 provides technology that improves reservoir storage efficiency while ensuring containment
- Tasks 2 and 3 provide methodology that supports industries’ ability to predict (or control) CO_2 storage capacity in geologic formations to within ±30 percent
- Task 4 develops technology to ensure 99% storage permanence

Project Overview Task 1:

Pressure Management Optimization Framework

- **Objectives**
  - Develop optimization framework for pressure management via optimized CO_2 injection and brine extraction (well placement and rates)
  - Define specific performance criteria (e.g., maximum pressure near fault zone, maximum leakage rate, maximum caprock pressure), and, via smart search algorithms, automatically optimize well locations and injection/extraction rates to meet performance criteria
- **Technical Status**
  - Developed efficient constrained global optimization methodology
  - Incorporated suite of forward simulators into optimization framework
  - Demonstrated use of optimization framework for realistic GCS systems
  - Currently expanding optimization framework to broader storage management applications and real-time control based on monitoring

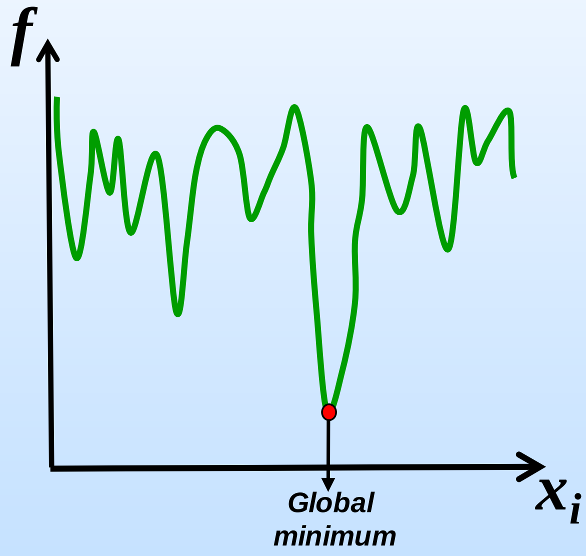
Example: Critically stressed fault



Task 1:

Efficient Global Optimization Strategies Needed for Large-Scale Pressure Management Problems

- Specifically for optimal well placement problems, due to complex reservoir geometry and heterogeneity in reservoir rock properties, objective functions tend to be highly irregular with multiple local optima in the solution space.
- The irregularity of objective functions can easily cause gradient-based methods to be stuck in a local minimum.
- Global optimization methods that involve derivative-free algorithms and stochastic search methods (e.g., evolutionary algorithms) are more suitable for solving the coupled optimal well placement and rate control problems.
- Global optimization methods require a large number of forward model runs; parallelization of the algorithms is essential but achievable.



Task 1:

Example Description of a Constrained Global Optimization Problem

A general constrained optimization problem for well placement, injection and extraction for maximum pressure control can be formally expressed as

Minimize $$f(\boldsymbol{x}_{ext}, \boldsymbol{y}_{ext}, \boldsymbol{p}) = \frac{V_{ext}}{V_{inj}}$$

Extraction Ratio (if no brine extraction, f is chosen as 1/V_{inj})

Subject to $$\Delta P_{th} - \max\left\{\Delta P\left(\boldsymbol{x}_f, \boldsymbol{y}_f, t\right)\right\} > 0$$

Pressure buildup constraints, e.g. max buildup along a fault

$$V_{ext,CO_2} = 0$$

No CO_2 flow into extraction wells (for brine extraction schemes)

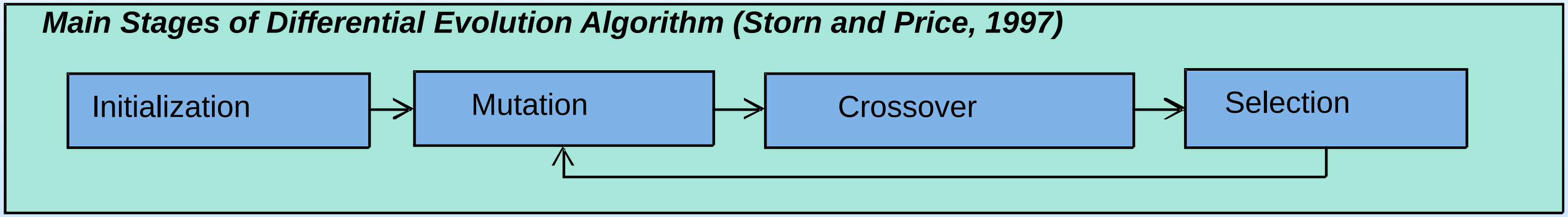
$$a_1 \le x_{inj,i} \le b_1,\ a_2 \le y_{inj,i} \le b_2$$

$$a_4 \le x_{ext,i} \le b_4,\ a_5 \le y_{ext,j} \le b_5$$

Range of Cartesian coordinates for vertical wells (for partially penetrating and horizontal wells, additional parameters can be included)

Task 1:
Constrained Global Optimization Methodology

- A constrained differential evolution (CDE) algorithm was developed for solving optimization problems involving well placement, injection, and brine extraction.
- The DE algorithm is a very powerful evolutionary algorithm with good convergence properties, ease of use and suitability for parallelization.
- The original DE method is in general applicable to unconstrained optimization problems.



Main Stages of Differential Evolution Algorithm (Storn and Price, 1997)

Implementation of Constraints in CDE

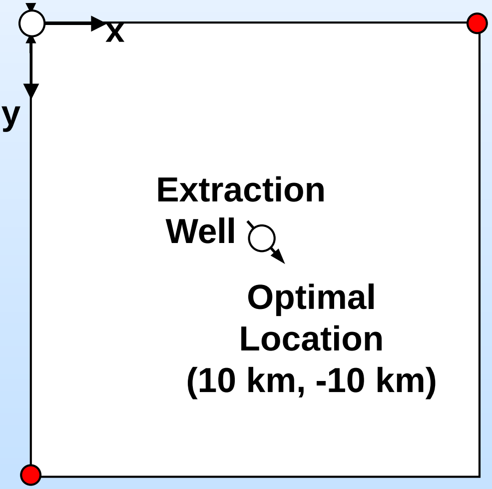
Objective function evaluations in the original DE is reformulated in the CDE based on the following criteria**:**

1. Any feasible (satisfying constraints) solution is preferred to any infeasible solution
2. Among feasible solutions, the one having the better objective function value is preferred
3. Among the infeasible solutions, the one having smaller constraint violation is preferred

Task 1:

Demonstration and Testing of Constrained Global Optimization Methodology

A Simple Optimization Problem with Known Optimal Extraction Well Location



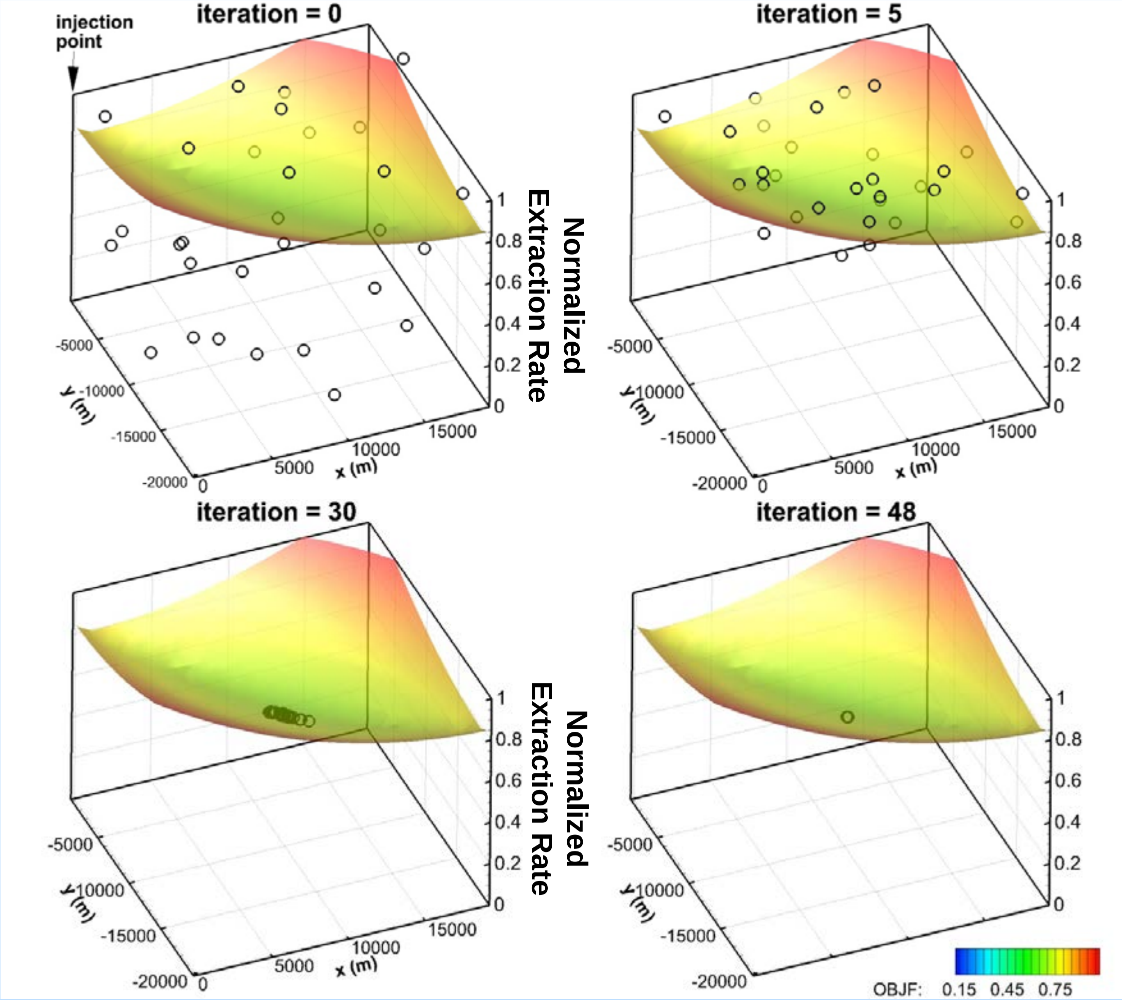
Injection Well
(x=0, y=0)

Impact Point
(x=20 km, y=0)
(Critical ΔP=0.2MPa)

Extraction Well

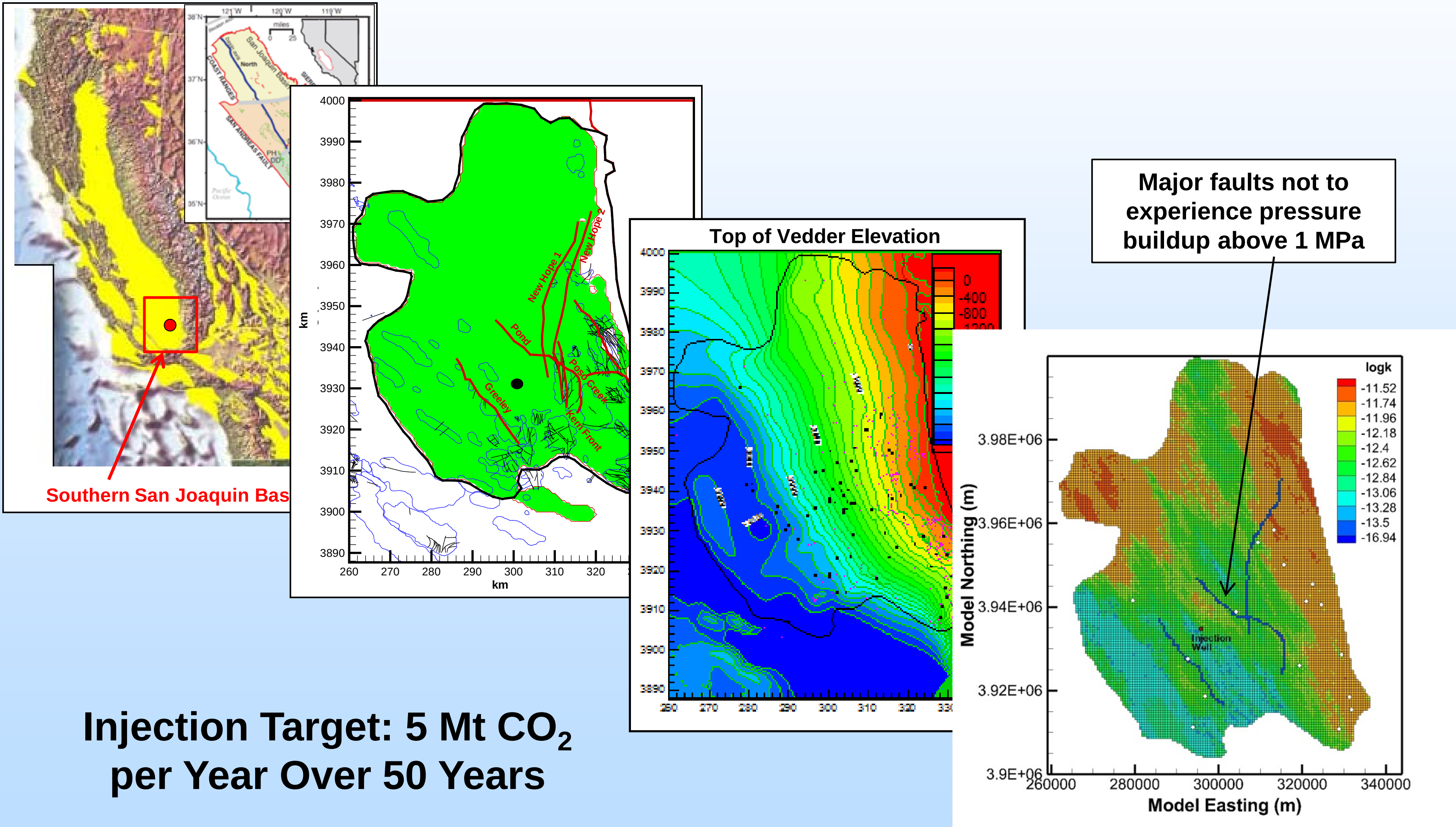
Optimal Location
(10 km, -10 km)

Impact Point
(x=0, y=-20km)
(Critical ΔP=0.2MPa)



Task 1:

Application to Hypothetical CO_2 Injection in the Vedder Formation (Southern Joaquin Valley, California)

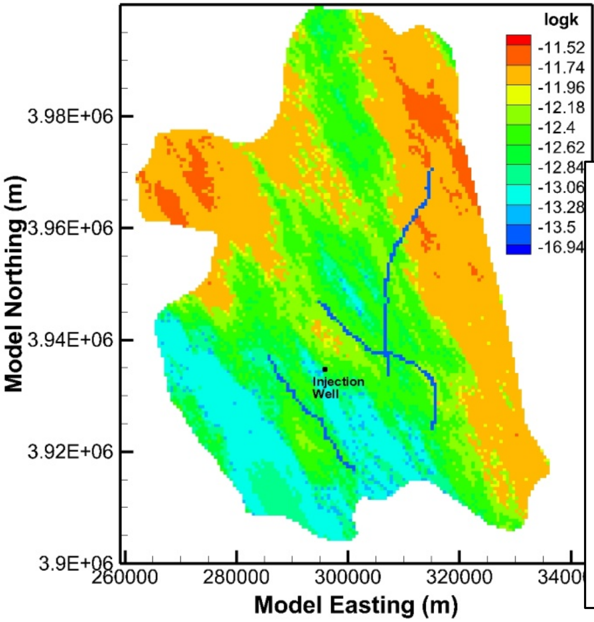


Major faults not to experience pressure buildup above 1 MPa

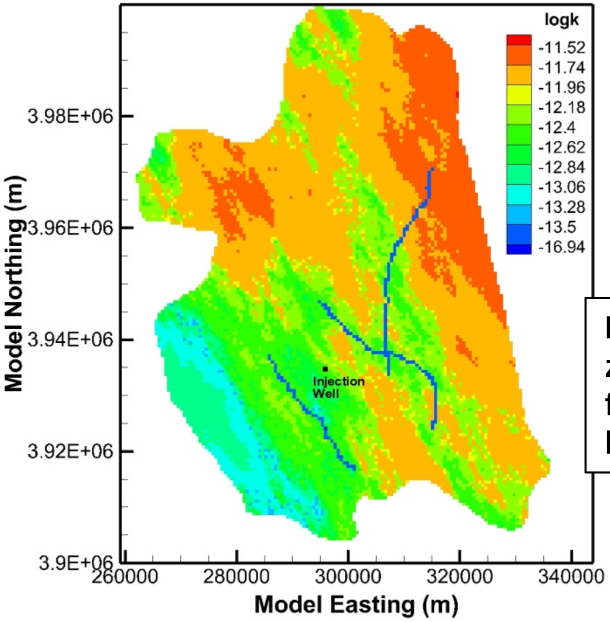
Injection Target: 5 Mt CO_2 per Year Over 50 Years

Task 1: Optimized Constant Injection Rates without Brine Extraction

Realization	Optimal Injection Rates without Brine Extraction for ΔP_{max}=1MPa along the Faults
1	1.968 Mt/yr
2	2.739 Mt/yr
3	3.229 Mt/yr
4	2.061 Mt/yr
5	2.451 Mt/yr



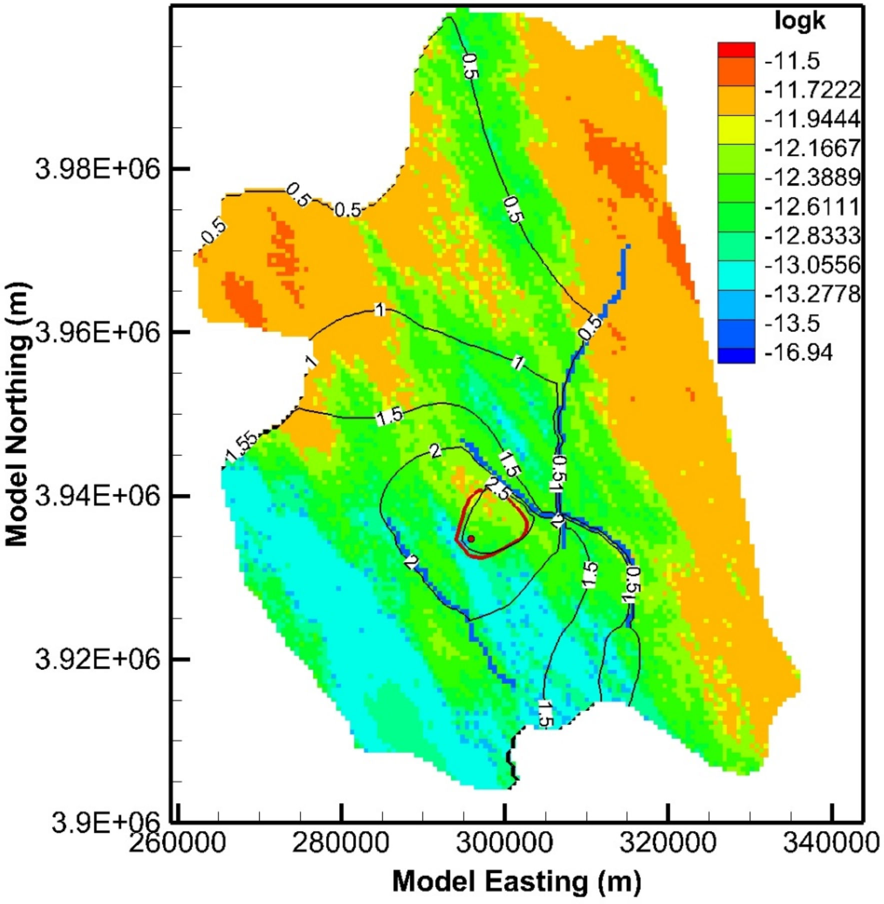
Lower permeability zones around the injection zone and in between the faults cause strong pressure buildup and thus low optimal injection rate without creating fault slippage.



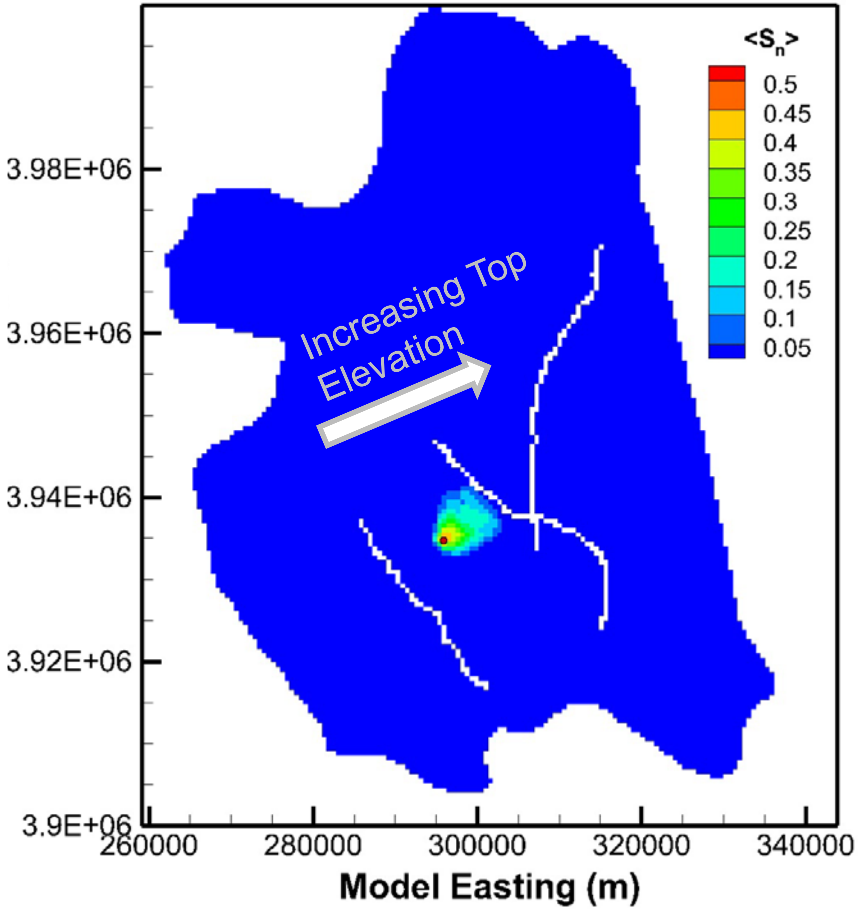
Higher permeability zones between the faults result in higher injectivity.

Task 1:

Results for Injection of 5 Mt CO_2 per Year Over 50 Years Without Pressure Management



Pressure-buildup contour lines (black) in MPa and CO_2 plume extent (red)

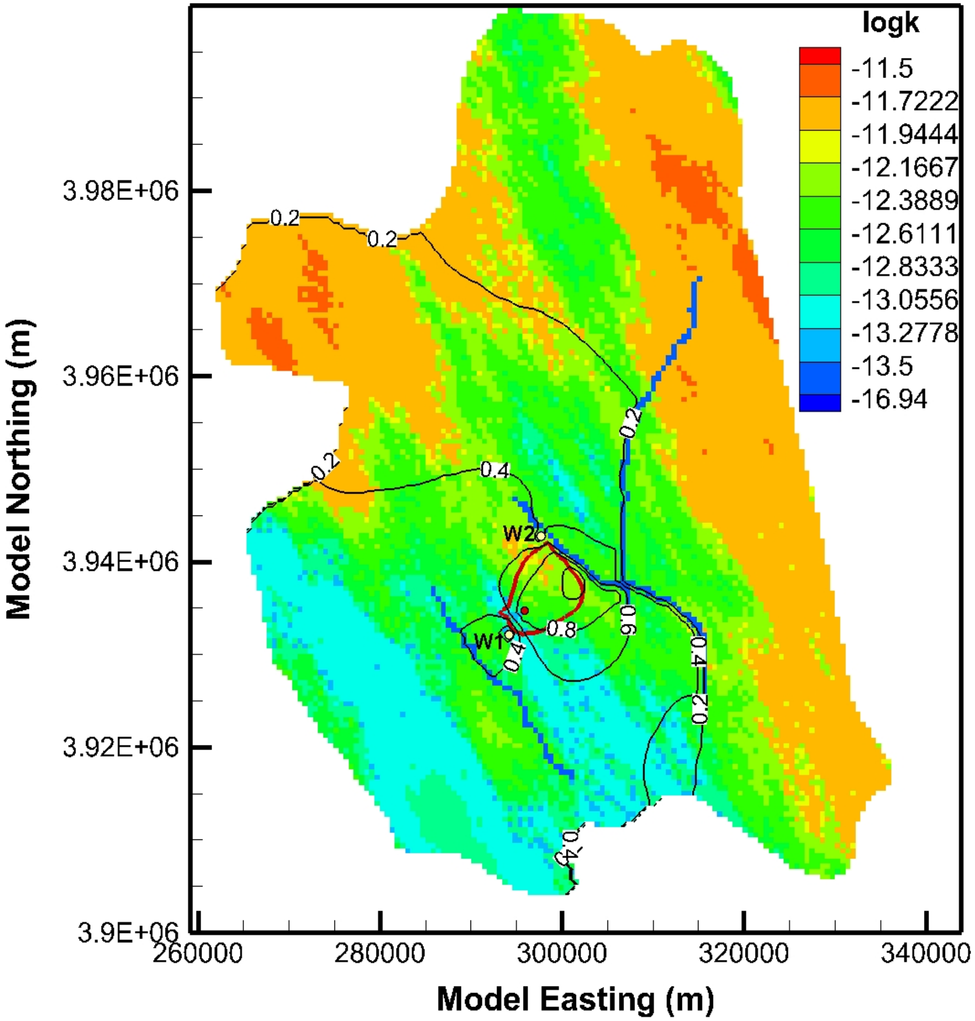


For Realization 1, at 50 years

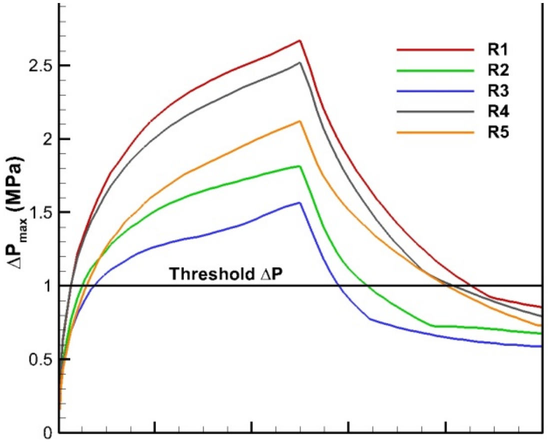
Task 1:

Optimal Well Placement and Pressure-Buildup Changes

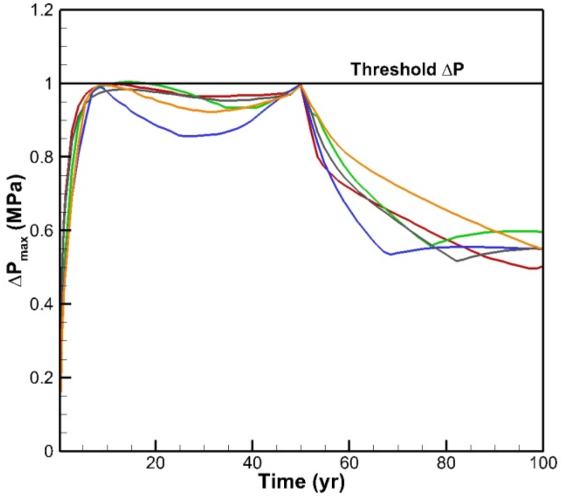
Results for Realization 1



Maximum Pressure Buildup Without Brine Extraction



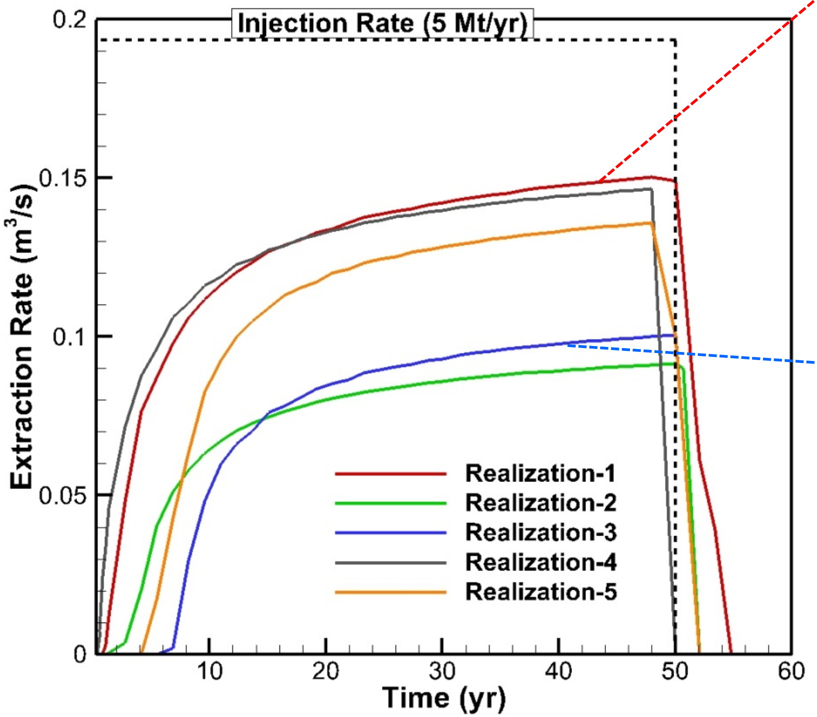
With Optimized Brine Extraction

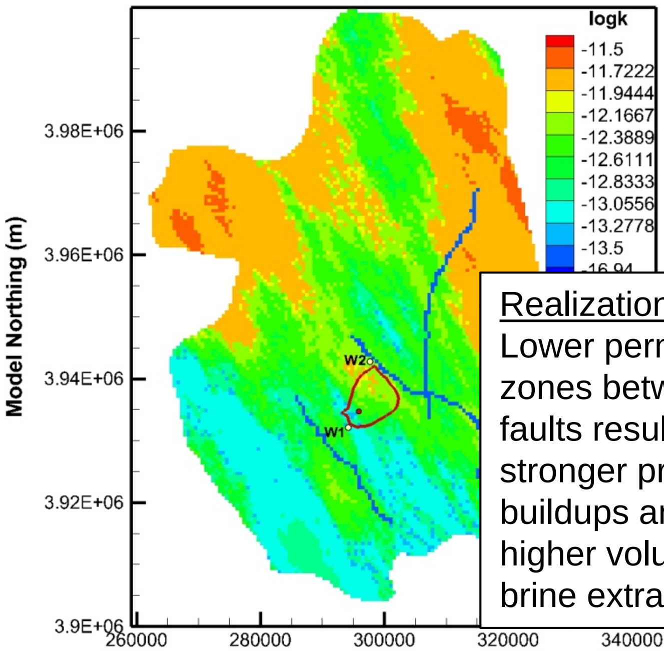


Task 1:

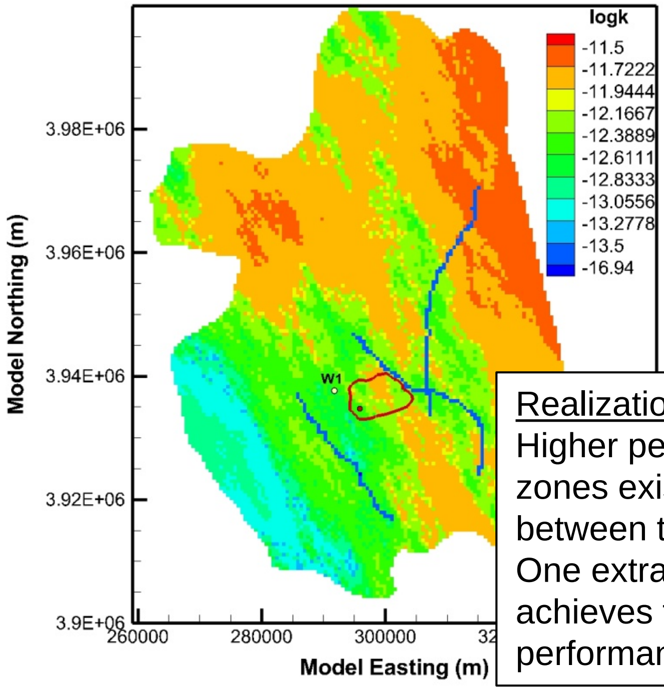
Heterogeneity plays a significant role for optimal well placement and extraction rate

R	Optimal Injection Rates without Brine Extraction for ΔP_{max}=1MPa along the Faults	Optimal Extraction Ratios for 5Mt/year injection and ΔP_{max}=1MPa along the Faults
1	1.968 Mt/yr	0.672
2	2.739 Mt/yr	0.393
3	3.229 Mt/yr	0.380
4	2.061 Mt/yr	0.654
5	2.451 Mt/yr	0.538





Realization-1
Lower permeability zones between the faults result in stronger pressure buildups and thus higher volume of brine extraction



Realization-3
Higher permeability zones exist between the faults. One extraction well achieves the performance goal

Project Overview Task 2:

Simulation Capabilities for GCS in Oil Reservoirs

- **Objectives**
  - To develop rigorous simulation capabilities for oil, natural gas, brine, and CO_2 systems within the framework of the TOUGH family of codes
  - These developed capabilities will be used for risk assessment, performance assessment, and long-term process modeling related to CO2-EOR

- **TOUGH2-CO2EOR**
  - Is a TOUGH2-based numerical simulator for modeling CO2-EOR processes
  - The general framework of the simulator has been acquired and adopted from a simulator developed at Colorado School of Mines (Di et al., 2011).
  - The modeling method is three-dimensional, three-phase (water, CO_2, and oil), non-isothermal, and compositional.
  - The SRK equation of state is used for estimating fluid properties, and a K-value approach is adopted for estimating the partitioning of oil components and CO_2 between oil and CO_2 phases.

Di, Y., Wu, Y.-S., Ju, B., Qin, J., Song, X. (2011), A practical compositional method for simulation of CO_2 flooding in porous and fractured petroleum reservoirs, SPE-145096-PP, SPE Asia Pacific Oil and Gas Conference and Exhibit, September 20-22, Jakarta, Indonesia.

Task 2:

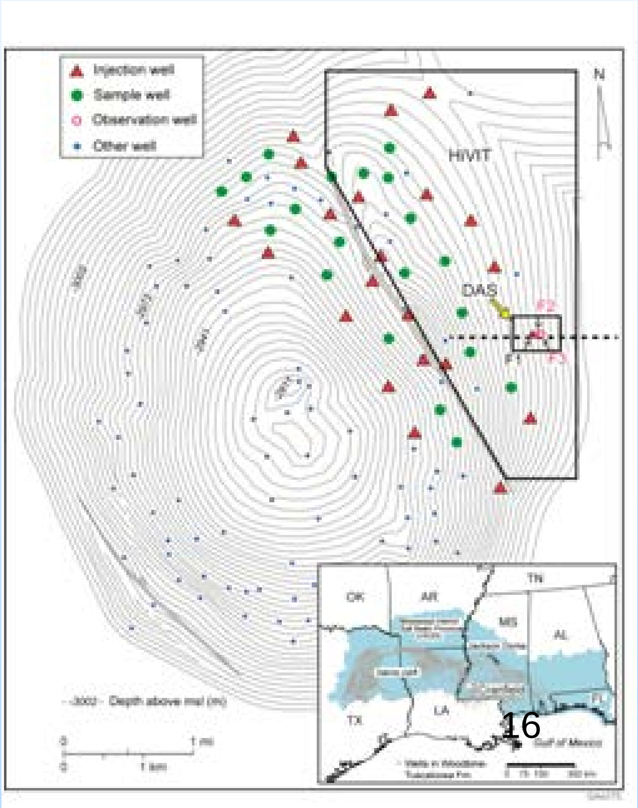
Simulation Capabilities for GCS in Oil Reservoirs

- **Technical Status**
  - The adopted version of the simulator is currently being upgraded and enhanced for developing it into a more general CO2-EOR simulator – some convergence issues along with other coding concerns are also being resolved.
  - Effort is also being directed towards better representation of processes (e.g., transition from two-phase to three-phase conditions; accurate estimation of properties of fluid mixtures under miscible and immiscible conditions; determination of the impact of CO_2 on oil properties including its relative permeability and capillary behavior).
  - A commercial simulator, COZSim[1], has been and implemented for benchmarking various aspects of TOUGH2-CO2EOR performance.

[1] http://http://www.niteclc.com/COZ_Download.html

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



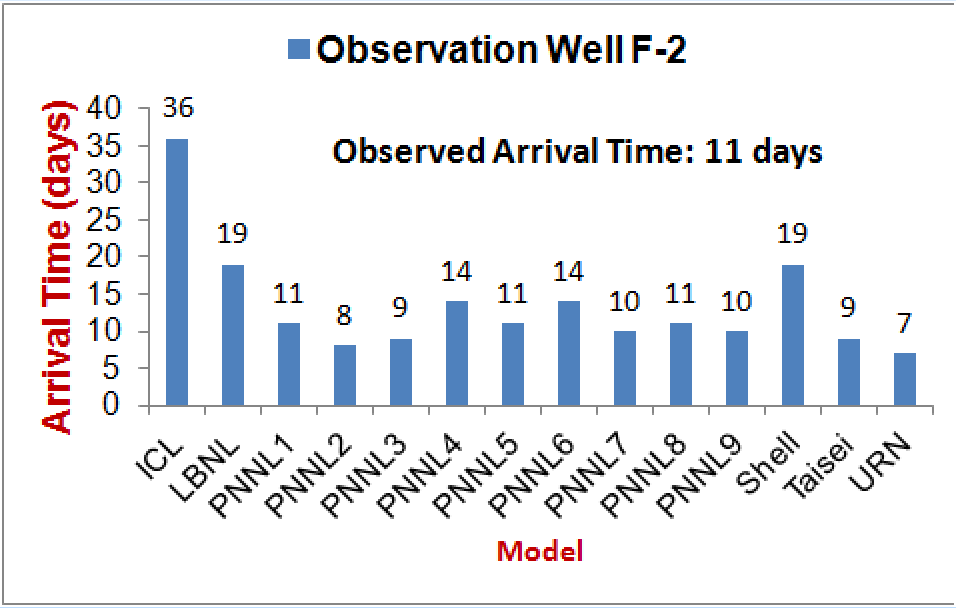
Location map of the S-3 site including the Detailed Area Study (DAS); Courtesy of JP Nicot

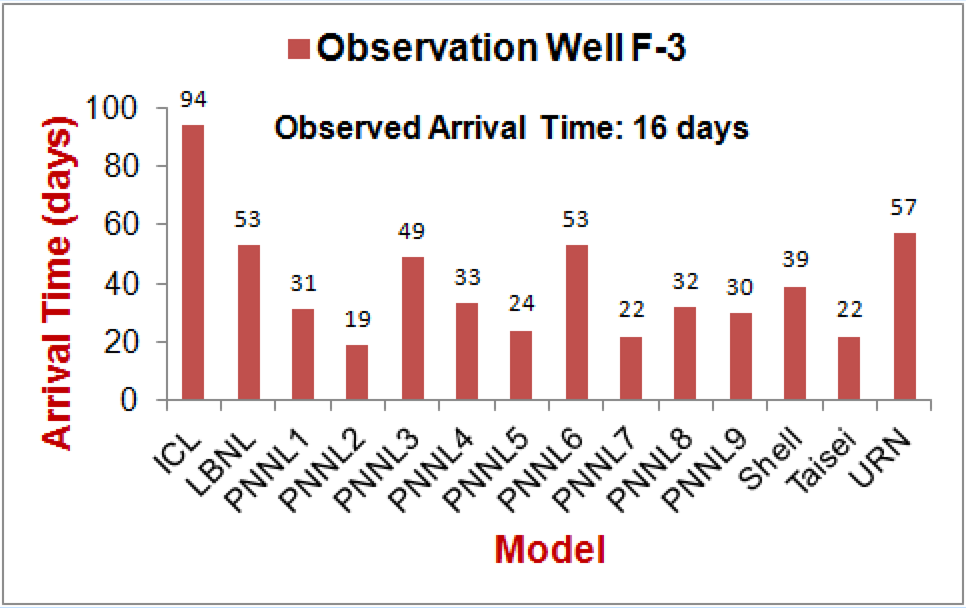
- **Technical Status**
  - Sim-SEQ currently involves 16 modeling teams from 8 countries
  - Modelers focus on one selected GCS field site, i.e., the S-3 site, patterned after the Phase III CO_2 injection project at Cranfield, MS
  - Predictive flow models have been developed and model-to-model comparison has been finalized
  - Model refinement using field observations and model-to-data comparison is ongoing

Task 3:

Sample Results from Model-to-Model Comparison

Acknowledgment: JP Nicot (BEG)

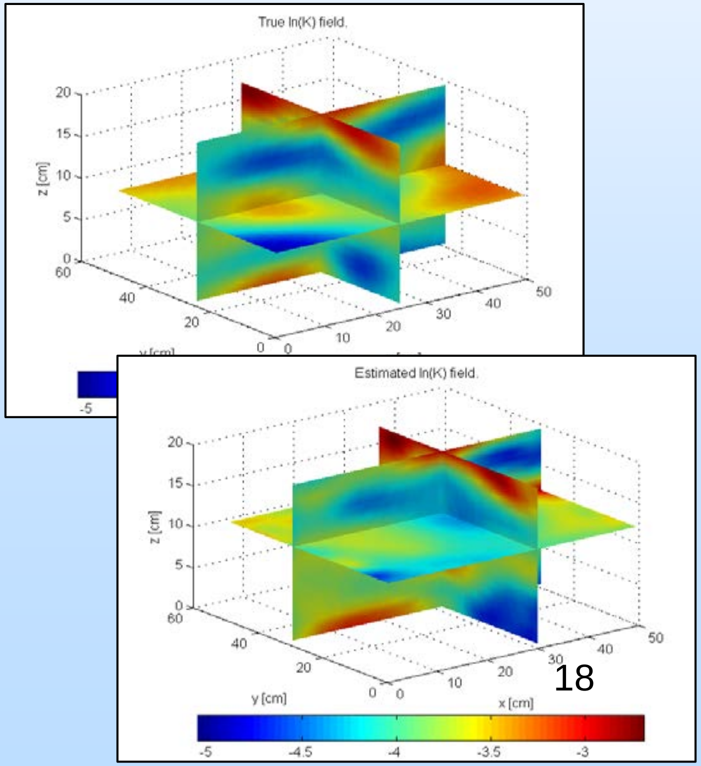




Project Overview Task 4:

Stochastic Joint Inversion for CO_2 Storage Modeling and Monitoring with Applications

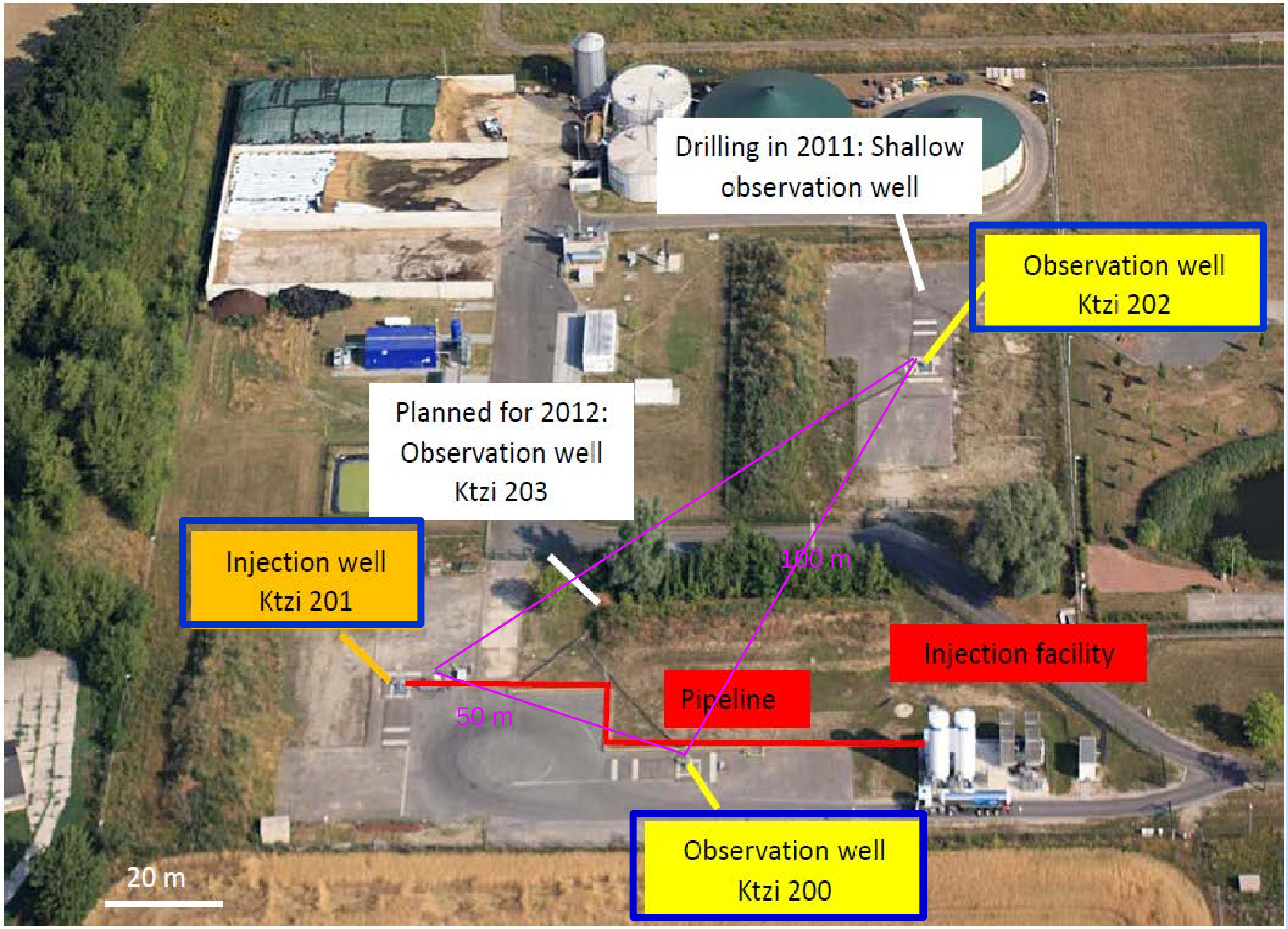
- **Objective**
  - Develop stochastic inversion methods as an efficient calibration tool for joint analysis of multiple types of uncertain and often very large data sets
  - Demonstrate applicability and use of new methods to pumping tests and CO_2 pilot injection test at the Ketzin site in Germany



- **Technical Status**
  - Developed efficient inversion framework using Krylov subspace methods and forward model model reduction (Liu et al., 2013, 2014)
  - Applied efficient stochastic inversion methods to Ketzin pumping tests for improved match with monitored pressures and improved geologic model
  - Currently applying the inversion tools to CO_2 injection test at Ketzin for further geologic model refinement

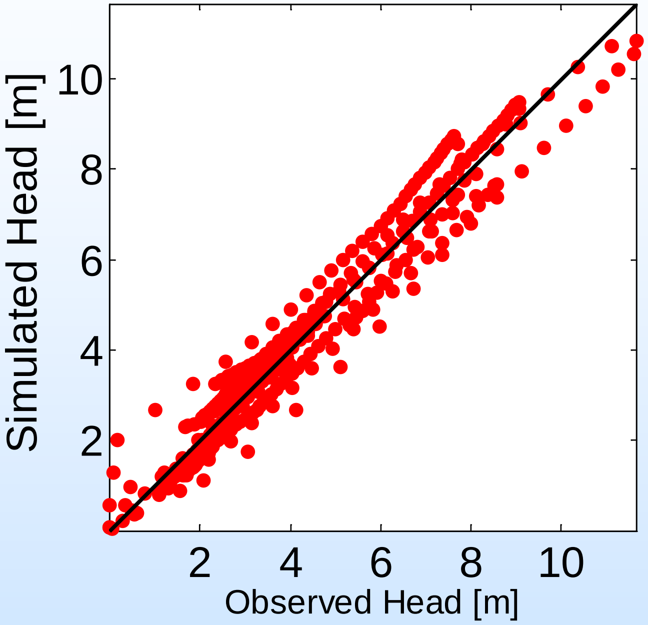
Task 4:

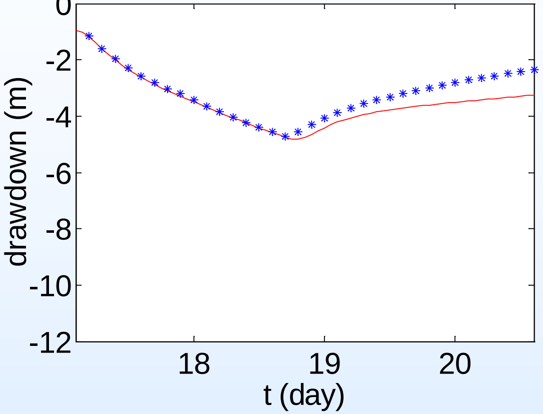
Ketzin Site Description

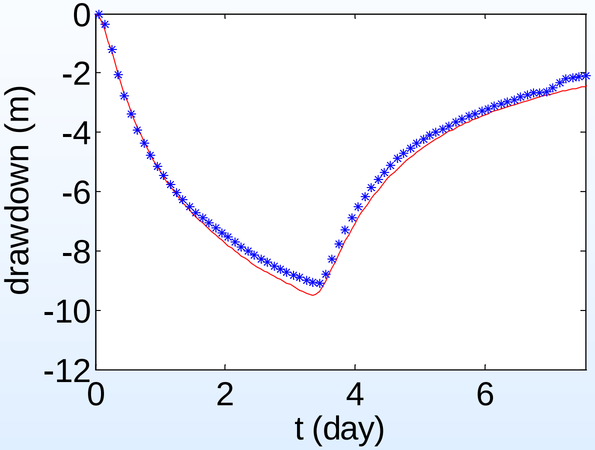


Task 4:

Pressure Results After Inversion


Overall Match


P200O201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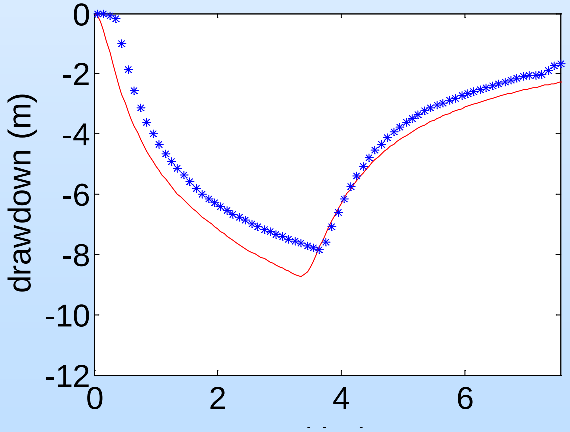
Good matches between observed (blue symbols) & inverted (red line) pressure change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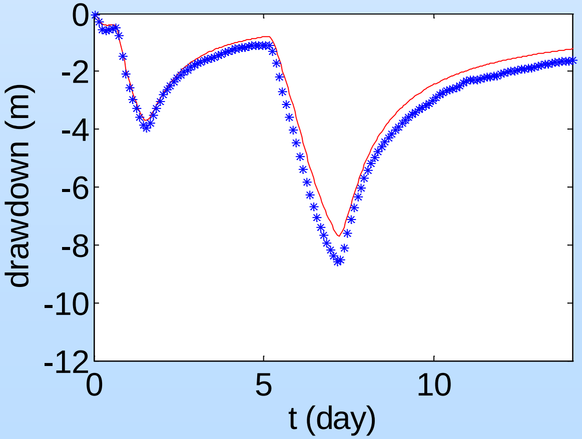
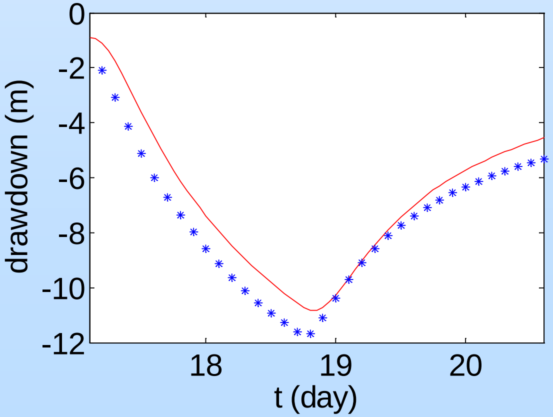

P201O202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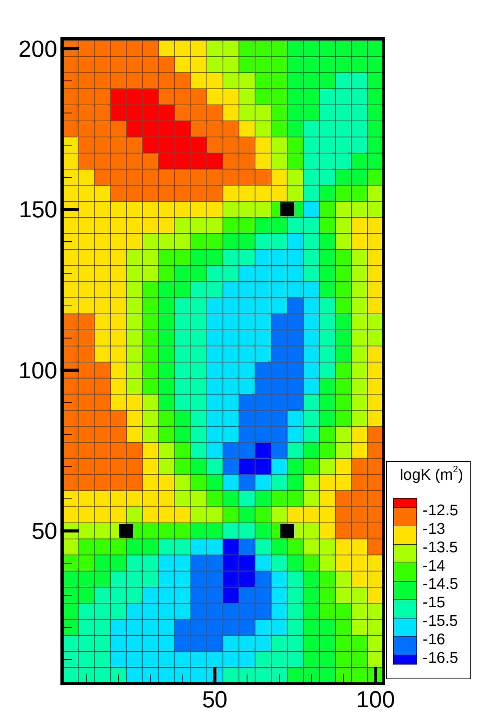
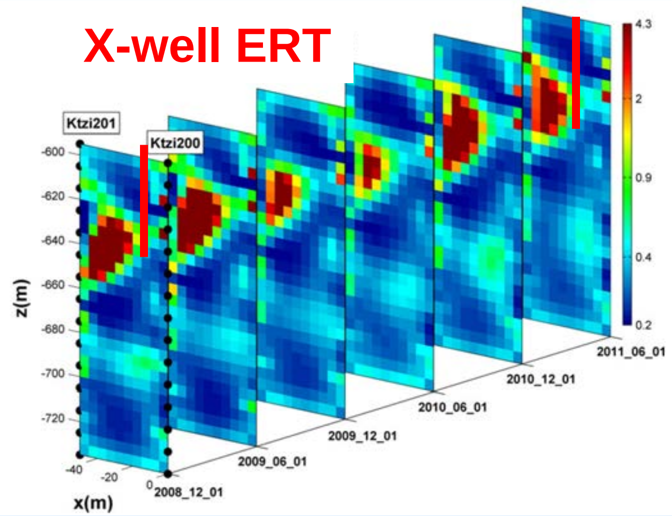
Task 4:

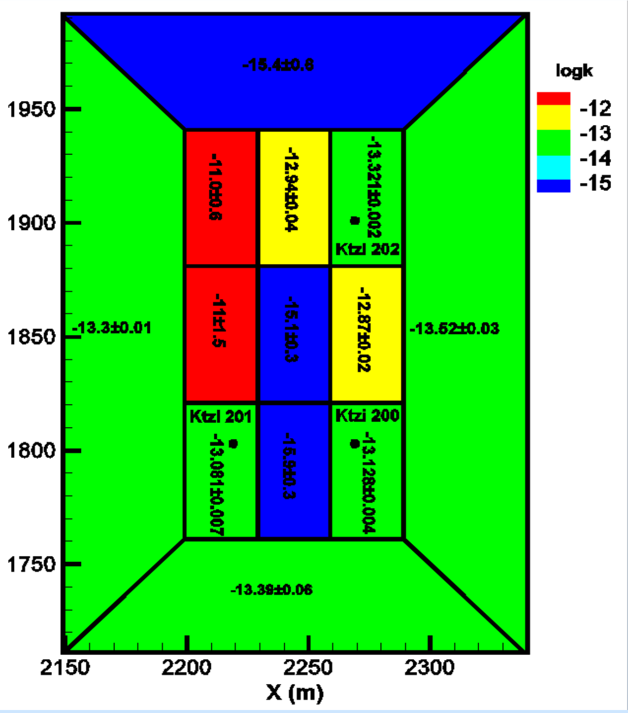
Permeability Fields After Inversion

Stochastic Inversion

iTOUGH2 Inversion







Chen et al., 2014

- 2D forward model with a non-uniform mesh covering 1.4 km × 1.4 km
- 2D permeability field with 21 × 41 unknowns in the pumping-affected area
- Inversion results show (1) a low-k barrier between 201 and 200, and (2) high-k channel between 201 and 202

- The inverted geologic features were also (1) evidenced from cross-well ERT data with different times and 3D seismic data in 2009 and 2011; and (2) inverted using 13 zones for upper high-k layer by iTOUGH2-PEST with deterministic inversion and a 3D forward model of 1327 2D cells × 24 layers.

Accomplishments to Date

- Task 1: Pressure Management Optimization Framework
  - Developed a new constrained global optimization framework for pressure management involving injection/extraction well placement and rates, and applied the global optimization methodology to realistic complex problems involving pressure control near faults and other management objectives
- Task 2: Simulation Capabilities for GCS in Oil Reservoirs
  - Based on an adopted CO2-EOR code from Colorado School of Mines, continued development and testing of TOUGH2-CO2EOR – a simulator for CO2-EOR within the TOUGH2 framework
- Task 3: Sim-SEQ Model Comparison Using Field Data
  - Built Sim-SEQ into a multi-national model comparison initiative with involvement of 16 international modeling teams
- Task 4: Efficient Methods for Stochastic Inversion
  - Applied the stochastic inversion tools developed in FY13 to pumping tests conducted at Ketzin pilot test to better characterize the spatial distribution of permeability of the highly heterogeneous Stuttgart Formation

Summary

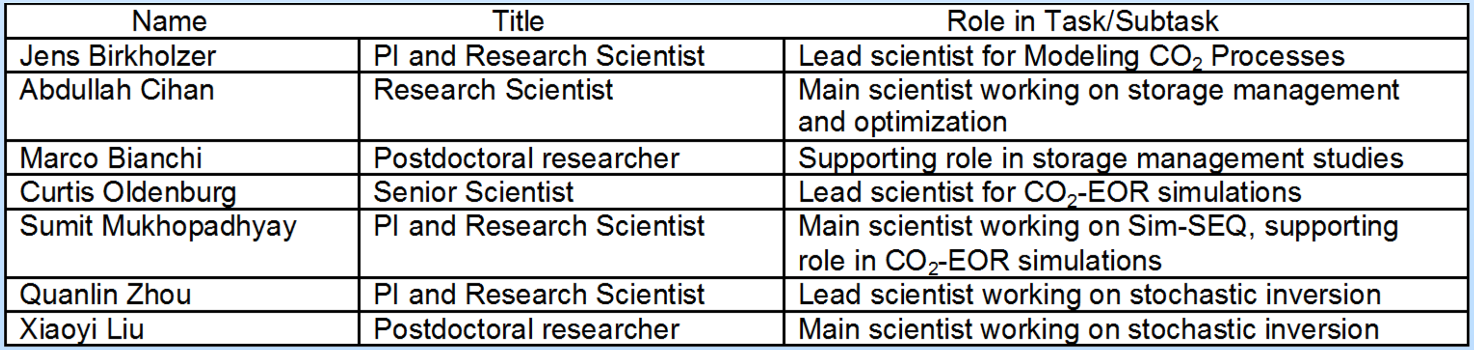
- **Key Findings / Lessons Learned from Modeling Tasks**
  - Task 1: The new constrained differential evolution algorithm is very well suited for solving complex and challenging storage management optimization problems
  - Task 2: The new CO2-EOR simulator is expected to become a useful addition in the TOUGH2 family of simulators
  - 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**
  - Long-term plan is to develop and demonstrate a broad and flexible GCS optimization framework for improved injectivity, permanence, monitoring, and utilization
  - This planned work builds on developments made in recent years, such as the advanced global and local search algorithms for pressure management, the new simulation capabilities for modeling GCS in oil reservoirs, and the advanced stochastic joint inversion methods for fast and intelligent analyses/processing of field data.
  - The optimization framework, including constrained global and local optimization methods, will allow for adaptive control, in the sense that storage management decisions will be revised in real-time using feedback from monitoring data.

Appendix

- These slides will not be discussed during the presentation, but are mandatory

Appendix: Organization Chart

- "Studies for Modeling CO_2 Processes" is a subtask of LBNL's Consolidated Sequestration Research Program
- "Studies for Modeling CO_2 Processes" has four main tasks with principal investigators identified as PI
  - Task 1: Abdullah Cihan, Marco Bianchi, and Jens Birkholzer (PI)
  - Task 2: Curtis Oldenburg (PI) and Sumit Mukhopadhyay
  - 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



Name	Title	Role in Task/Subtask
Jens Birkholzer	PI and Research Scientist	Lead scientist for Modeling CO_2 Processes
Abdullah Cihan	Research Scientist	Main scientist working on storage management and optimization
Marco Bianchi	Postdoctoral researcher	Supporting role in storage management studies
Curtis Oldenburg	Senior Scientist	Lead scientist for CO_2-EOR simulations
Sumit Mukhopadhyay	PI and Research Scientist	Main scientist working on Sim-SEQ, supporting role in CO_2-EOR simulations
Quanlin Zhou	PI and Research Scientist	Lead scientist working on stochastic inversion
Xiaoyi Liu	Postdoctoral researcher	Main scientist working on stochastic inversion

Appendix: Gantt Chart for FY14

Fiscal Year	FY14			
Task/Milestone **Quarter**	**Q1**	**Q2**	**Q3**	**Q4**
Task 1: Pressure Management Optimization Framework				
Incorporate Higher-Fidelity Simulators into the Optimization Framework	■			
Test Global Optimization Algorithms		■		
Apply IDPM Methodology to a Realistic Field Site			■	■ **H**
Task 2:Simulation Capabilities for GCS in Oil Reservoirs				
Development and acquisition of CO2-EOR simulation capabilities	■	■		
Implementation and debugging of TOUGH2-CO2EOR			■	■ **I**
Task 3: Sim-SEQ Model Comparison Using Field Data				
Perform Model-to-Model Comparison	■	■	■	
Perform Model-to-Data Comparison		■	■	■
Task 4: Efficient Methods for Stochastic Inversion of Uncertain Data Sets				
Develop Stochastic Joint Inversion Methods	■	■		
Develop Model Reduction Methods for Improved Computational Efficiency			■	■
Methodology Demonstration Using Synthetic Data				■

Appendix: Milestone Log for FY14

Task 1: Optimization of Brine Extraction for Pressure Management and Mitigation

- Milestone 4-1 (H), Q4 (9/30/14)
  Title: Development and Design of Storage Management Optimization Methodology

Task 2: Simulation Capabilities for GCS in Oil Reservoirs

- Milestone 4-2 (I), Q4 (9/30/14)
  Title: Report on testing and applications of CO_2-EOR simulations related to long-term trapping and fate of CO_2 during and after CO_2-EOR activities

Task 3: Sim-SEQ Model Comparison Using Field Data

- No milestone in FY14

Task 4: Methods for Stochastic Inversion of Uncertain Data Sets

- No milestone in FY14

Appendix: Bibliography 2008-2014

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