Studies for Modeling CO_2 Processes: Pressure Management, Basin-Scale Models, Model Comparison, and Stochastic Inversion

ESD09-056

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Developing the Technologies and
Infrastructure for CCS

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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

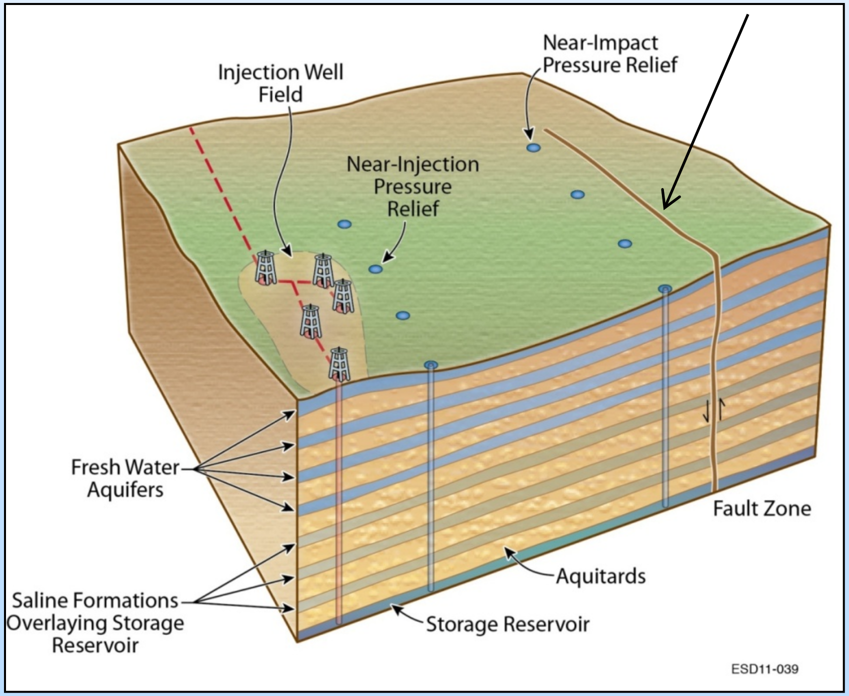
- Task 1 provides technology that improves reservoir storage efficiency while ensuring containment
  - This task develops optimization methods, and associated simulation tools, to design pressure management solutions at minimal cost
- Tasks 2 and 3 provide methodology that supports industries' ability to predict (or control) CO_2 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



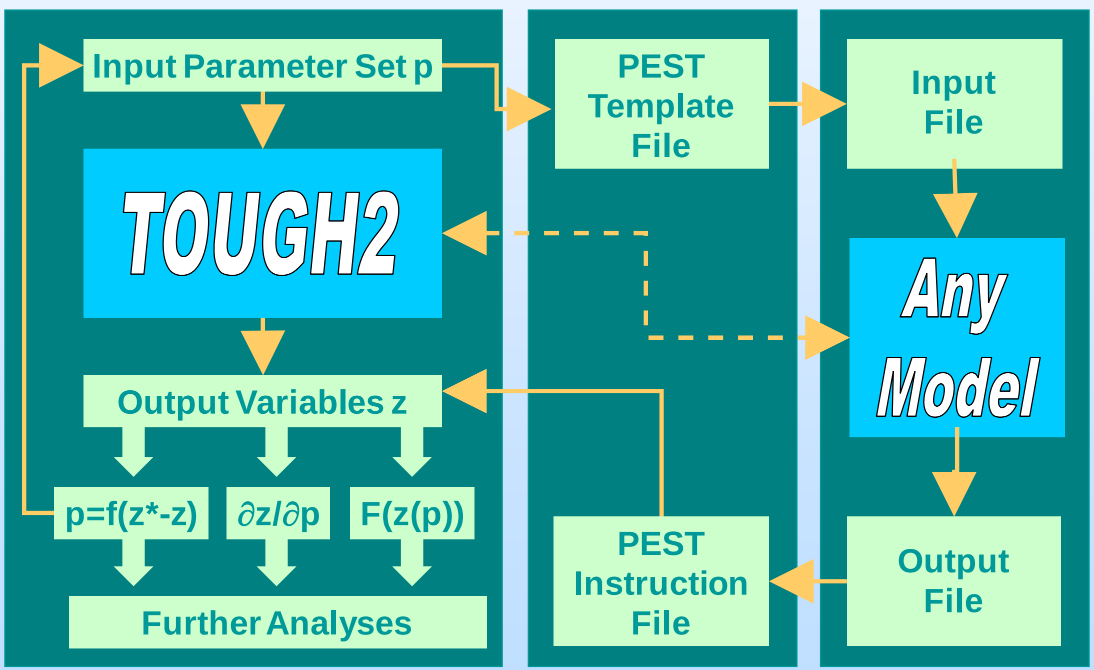
Technical Status Task 1:
Optimization of Brine Extraction for Pressure Management and Mitigation

- **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, CO_2 breakthrough)**
  - **IDPM optimization of one real CO_2 sequestration site**
- **Expansion of Optimization Method to Storage Management (FY14)**
  - Design and demonstrate storage management optimization for improved injectivity and enhanced CO_2 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

Increasing Realism

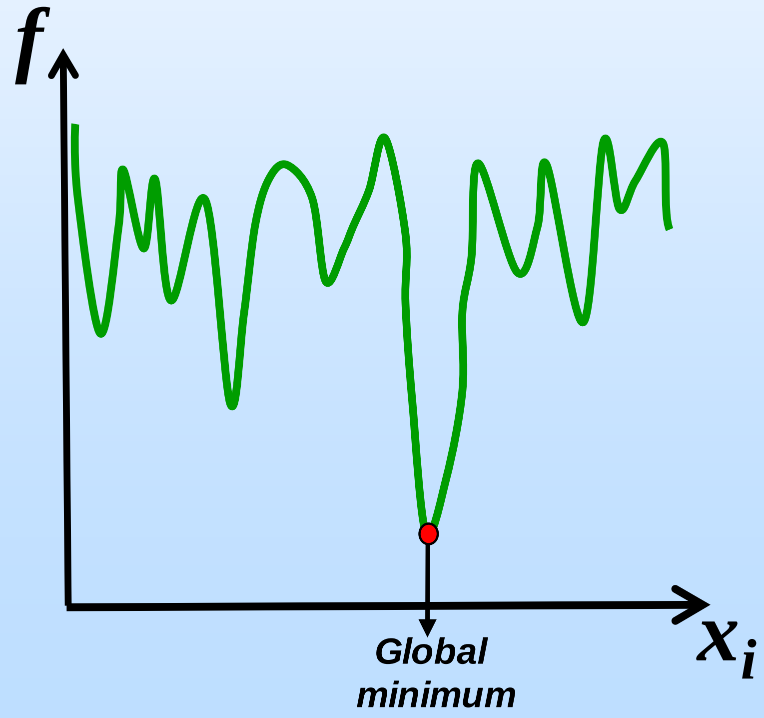
Increasing Efficiency

- (1) Analytical Solution
  - Single-phase flow in homogeneous infinite multi-layer systems
  - No CO_2 migration
- **(2)** Simulators Based on Vertical Integration
  - Sharp-Interface Models
  - **Vertically Integrated Multi-Phase Models**
  - CO_2 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 inverted for, rather than stepwise rates)

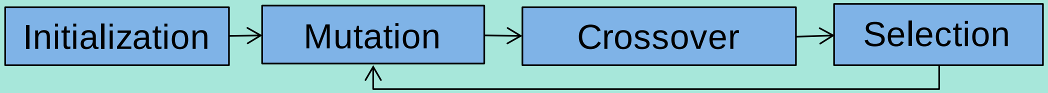
Differential Evolution Algorithm (DEA)

- ***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 CO_2 plume***

Levenberg-Marquardt Algorithm, (LM)

- ***Use LM to estimate optimum time-dependent actual extraction rates satisfying performance criteria.***

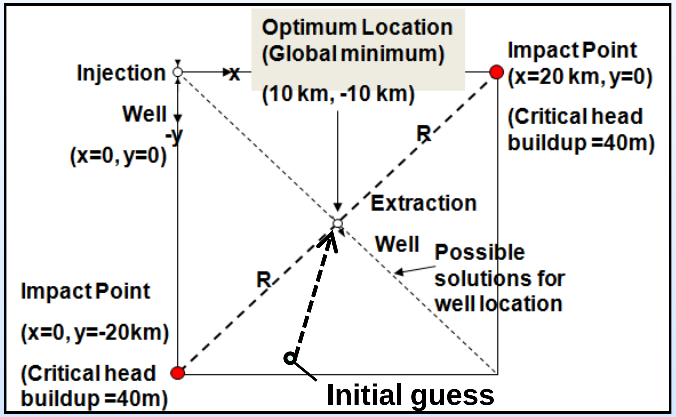
Main Stages of Differential Evolution Algorithm (Storn and Price, 1997)

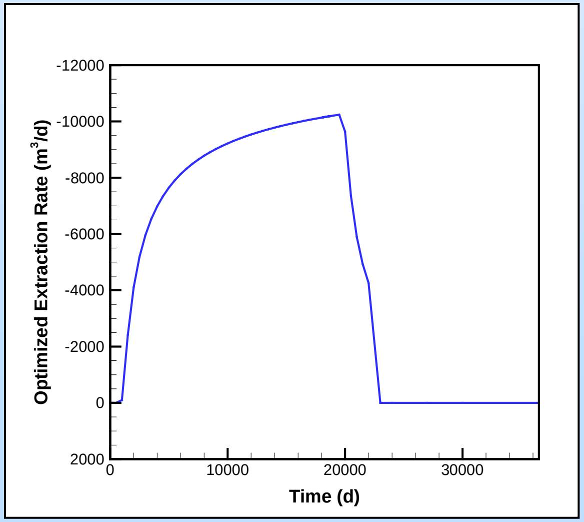


Task 1:

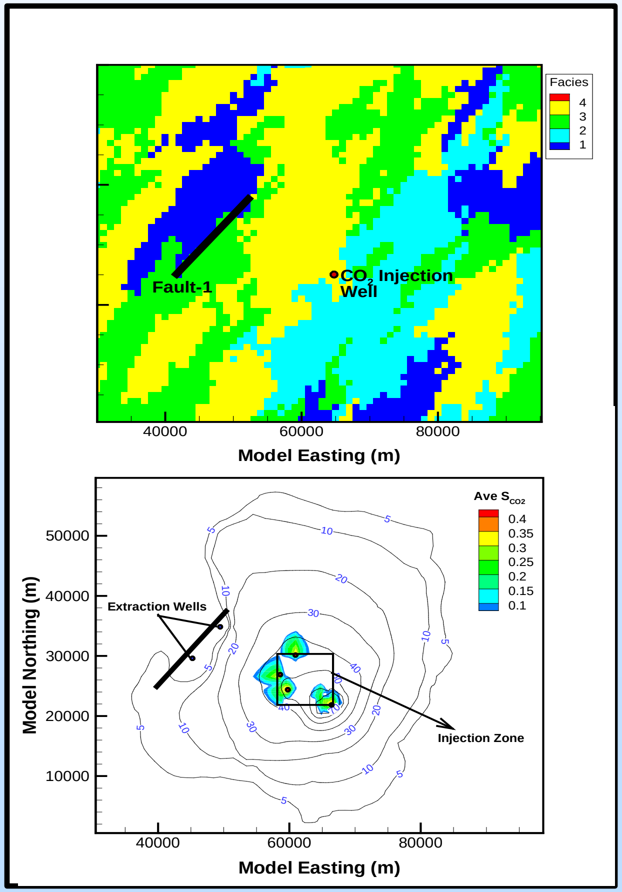
Verification of Solution Accuracy and Efficiency

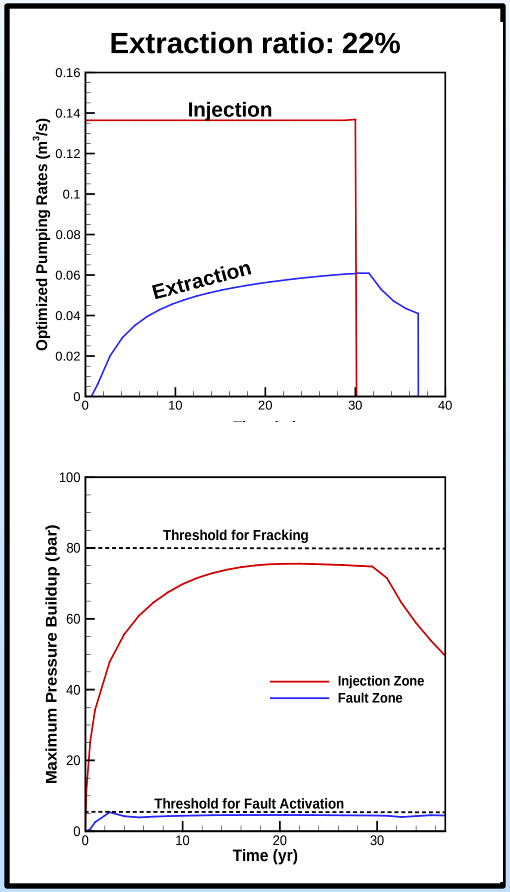
Test Problem 1: Verification against a problem with known solution. Two-step method reached the correct solution.





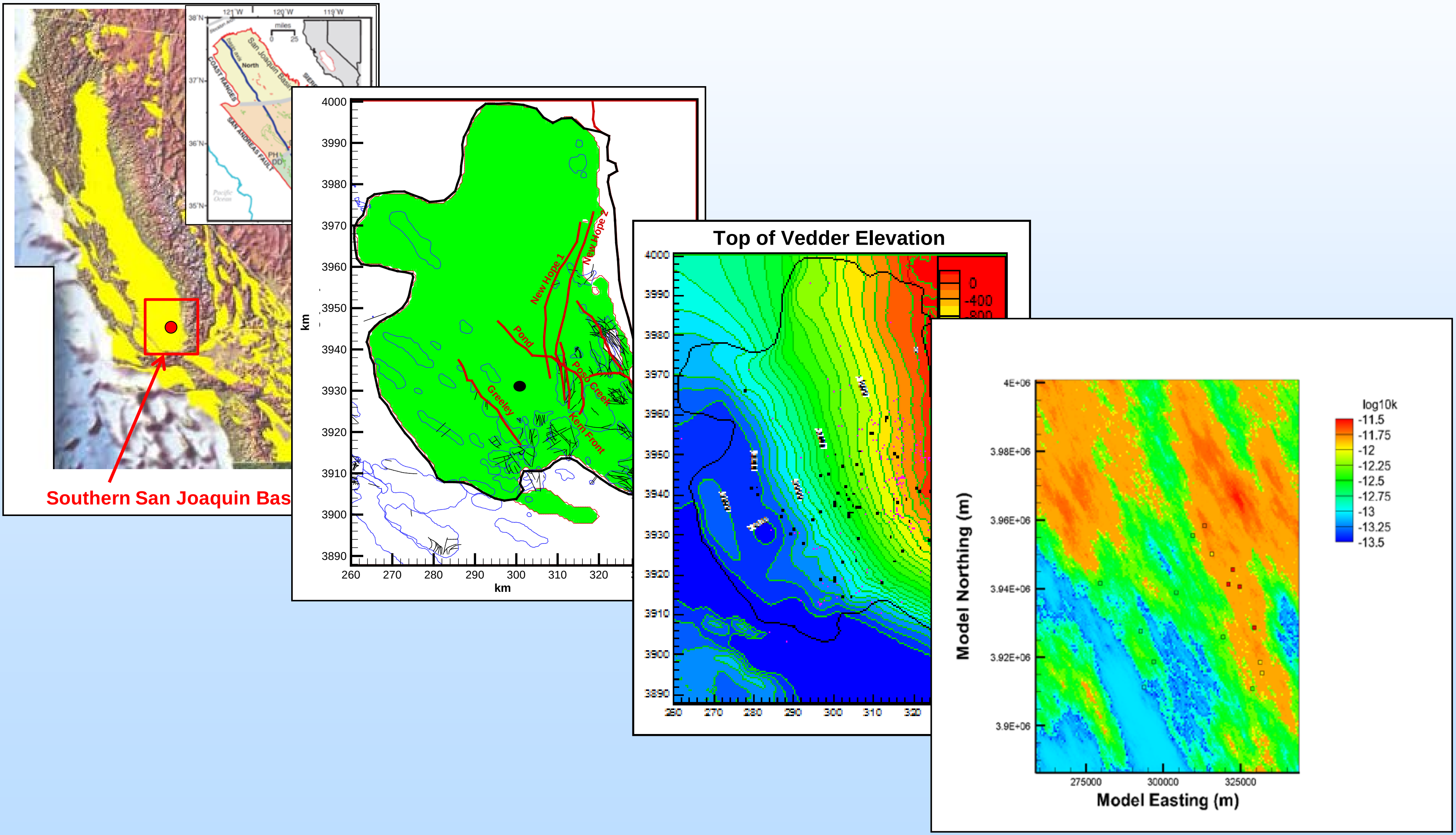
Test Problem 2: A scenario with heterogeneity and multiple injection wells near a fault. DEA and LM are used sequentially to optimize well placement, injection rates, and extraction rates for preventing fracturing and fault reactivation.





Task 1:

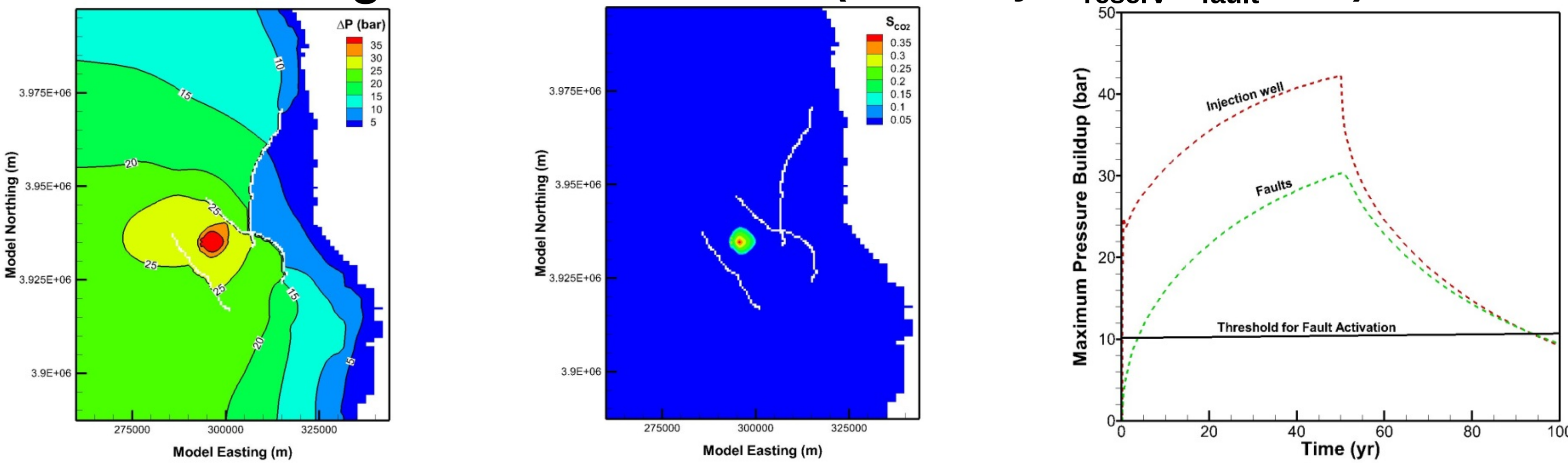
Application of IDPM for CO_2 Injection in the Vedder Formation (Southern Joaquin Valley, California)



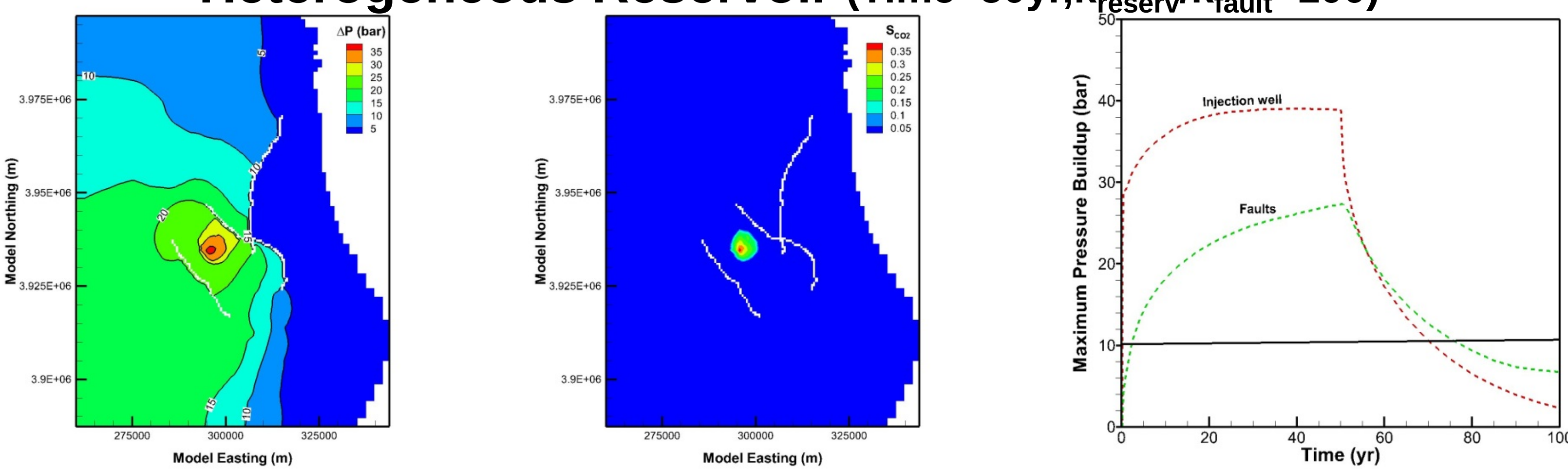
Task 1:

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

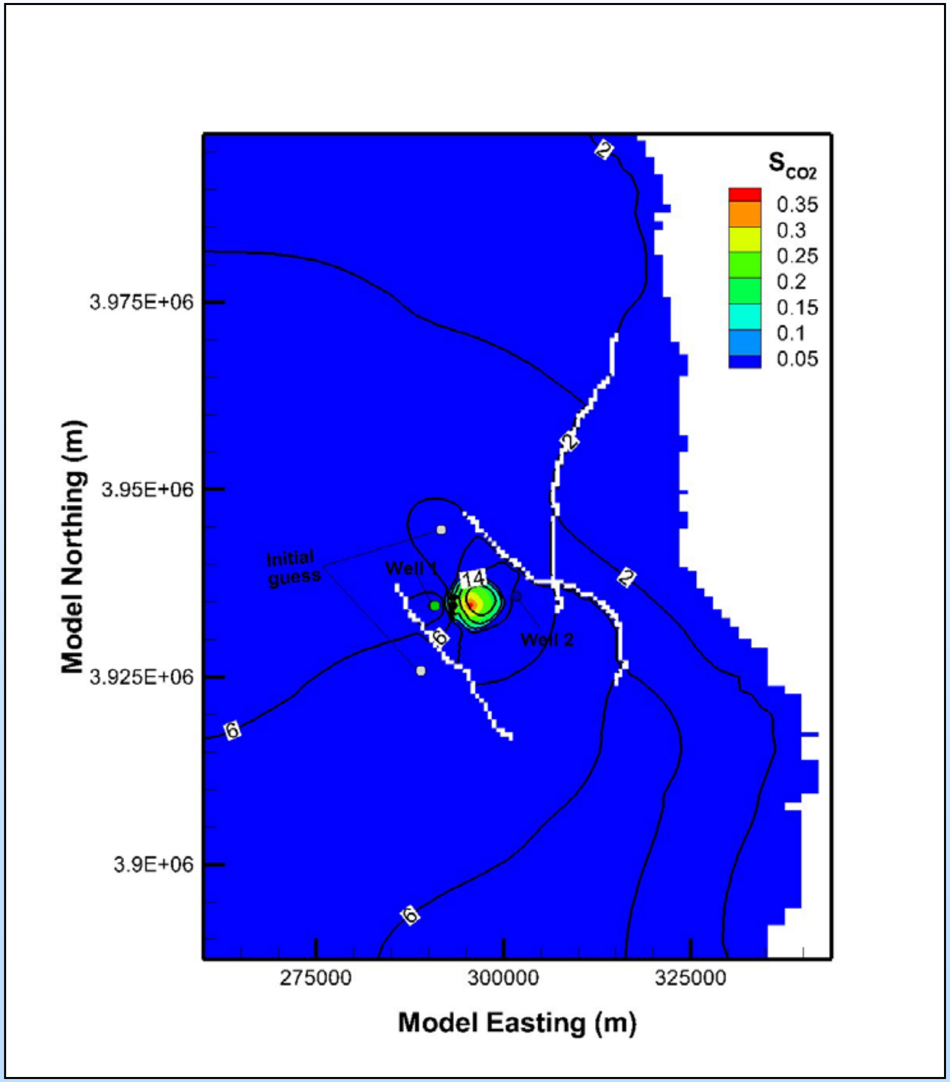
Homogeneous Reservoir (Time=50yr,k_{reserv}/k_{fault}=100)

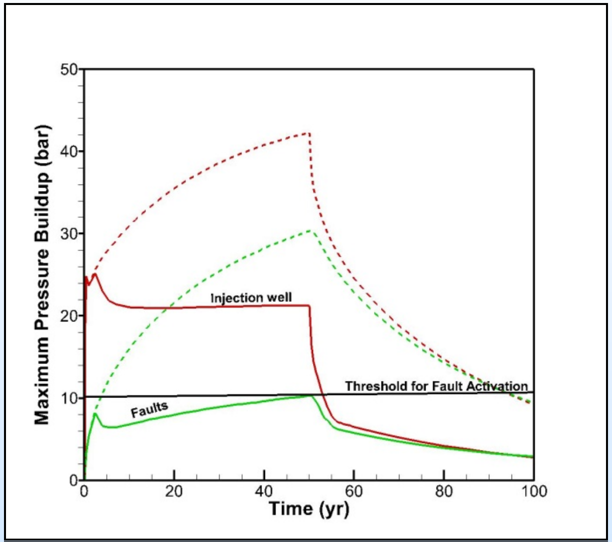


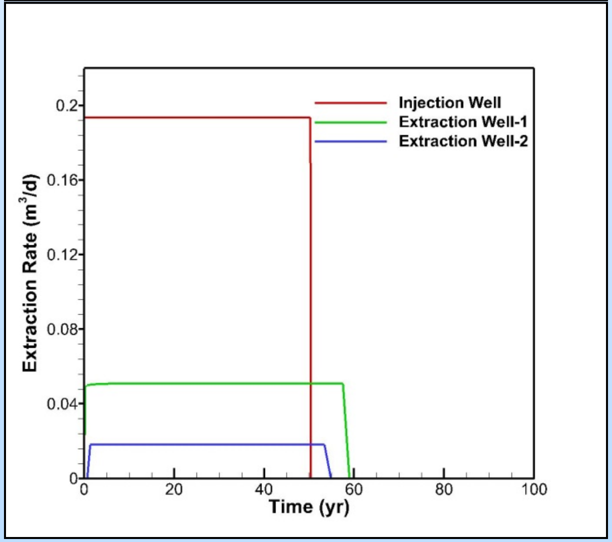
Heterogeneous Reservoir (Time=50yr,k_{reserv}/k_{fault}=100)



Task 1:
Optimized Well Placement and Extraction Rates for Homogeneous Scenario

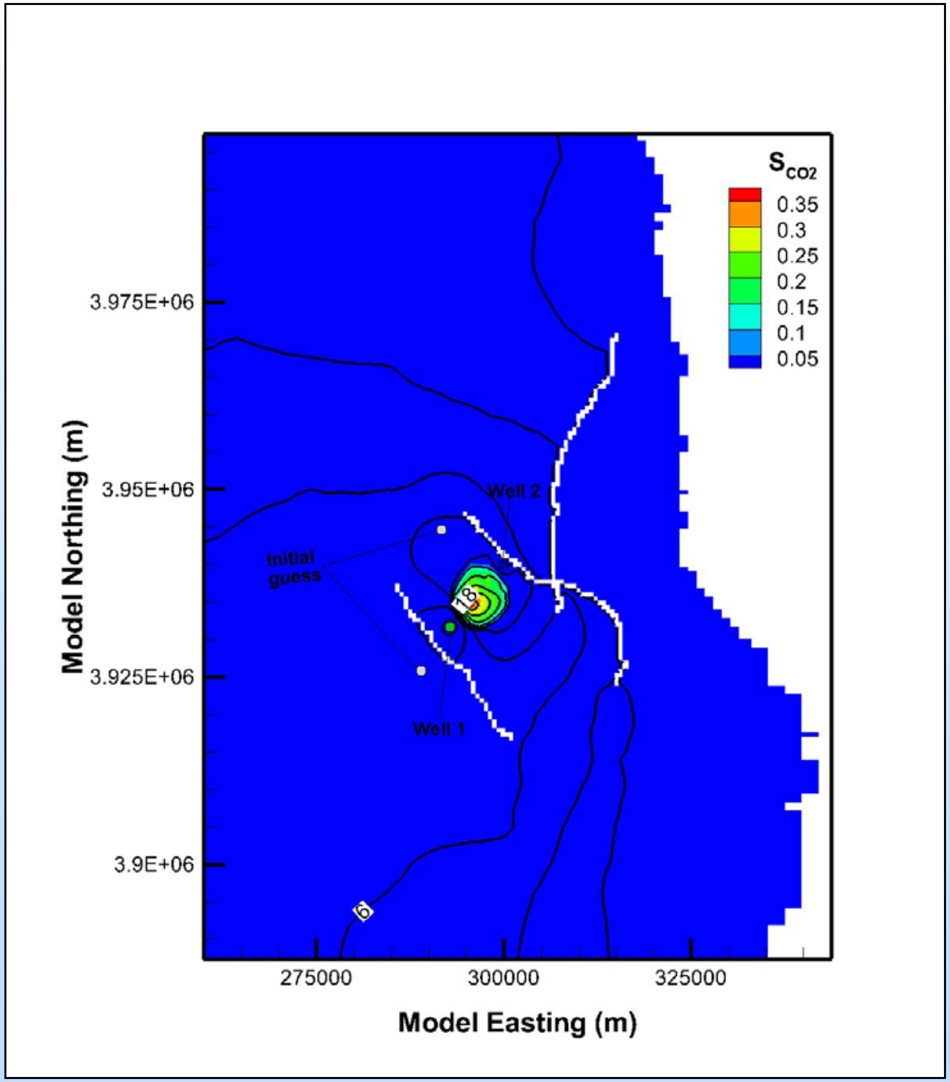


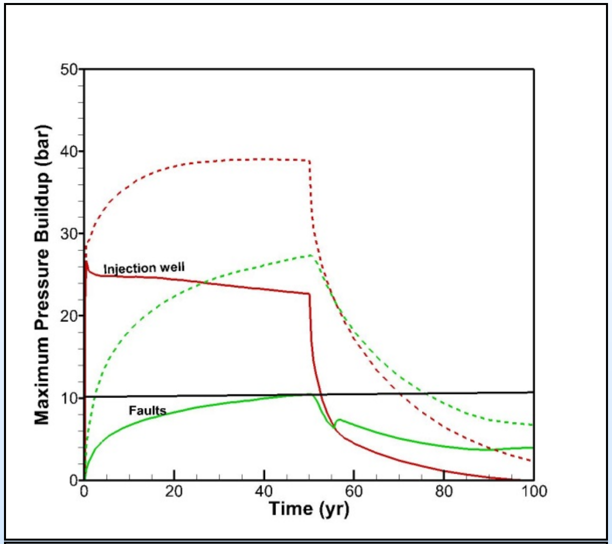


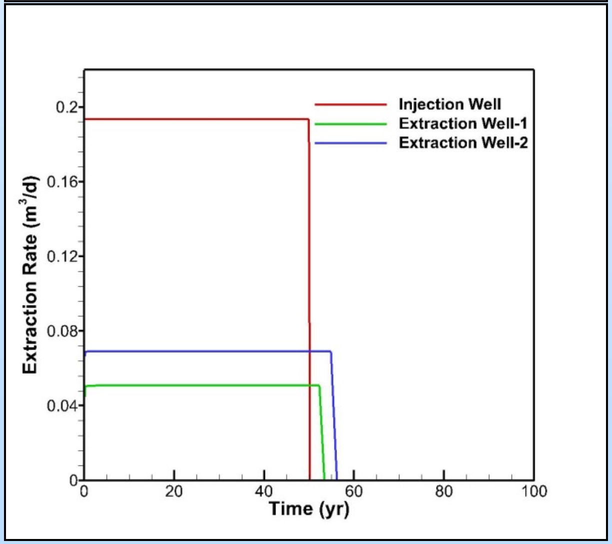


Task 1:

Optimized Well Placement and Extraction Rates for Heterogeneous Scenario







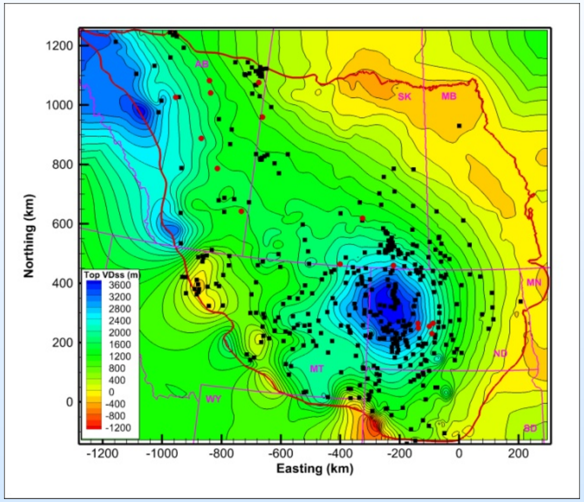
Project Overview Task 2:

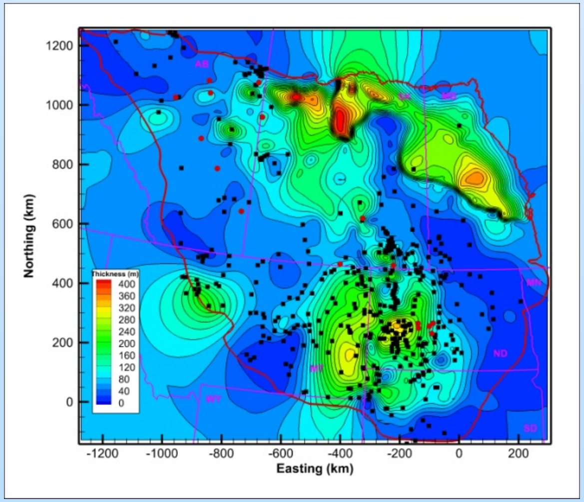
Basin-scale Simulation of CO_2 Storage in the Northern Plains – Prairie Basal Aquifer

- **Objective**
  - Conduct high-performance regional-scale simulations of future CO_2 storage scenarios in the Northern Plains – Prairie Basal Aquifer (Alberta and Williston Basin)
    - determine the distribution, migration, and long term fate of multiple CO_2 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 CO_2-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 CO_2 injections; comparison with simpler solutions is ongoing

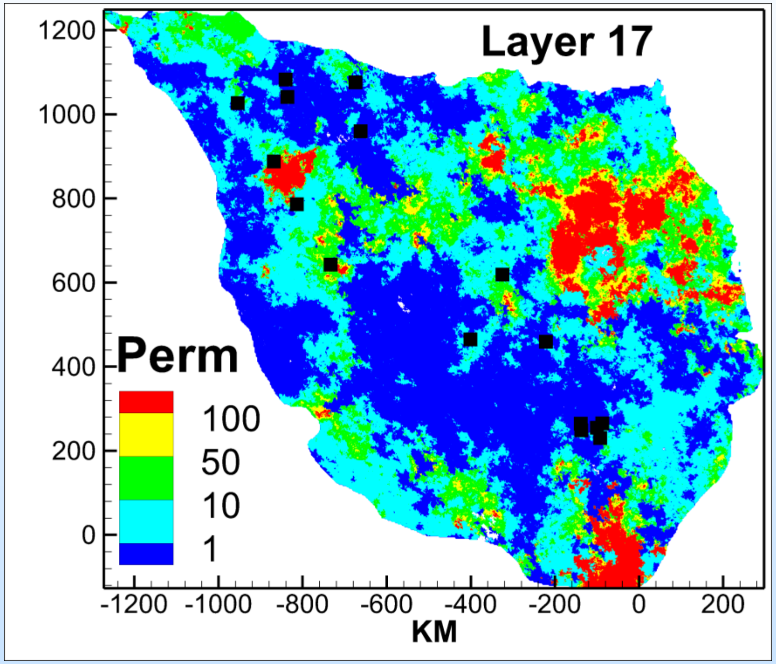
Task 2:
3D Geologic Model for the Basal Aquifer

Top Elevation and Thickness

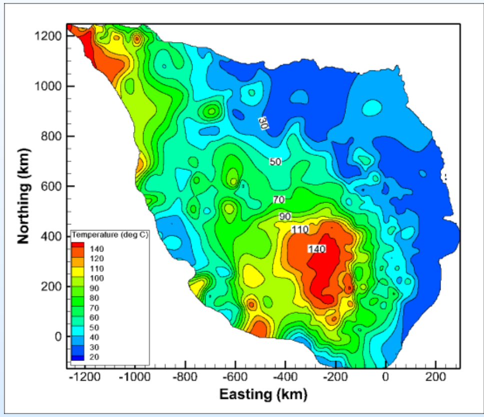


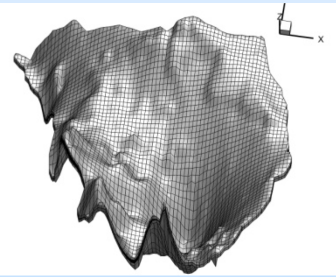


Porosity/Permeability



In Situ P/T/X





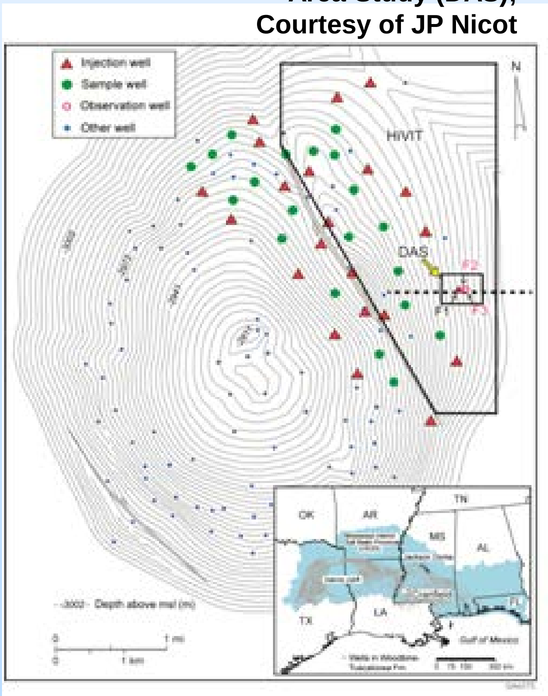
- EERC/AITF collected all well data in the Alberta Basin and the Williston Basin covering the model domain
- The Basal Aquifer consists of 25 model layers
- Porosity/permeability in all layers was generated using geostatistical approach with conditioning

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 CO_2 storage are sufficiently well understood

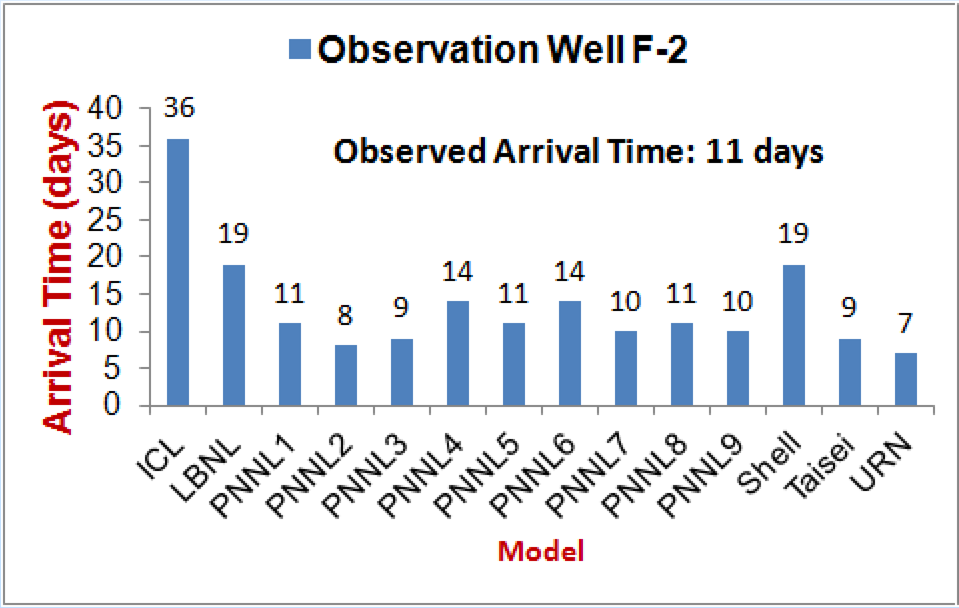
- **Technical Status**
  - Sim-SEQ currently involves 16 modeling teams from 8 countries
  - Modelers are at present focusing on one selected GCS field site, i.e., the S-3 site, patterned after the Phase III CO_2 injection project at Cranfield, MS
  - Predictive flow models have been developed and model-to-model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

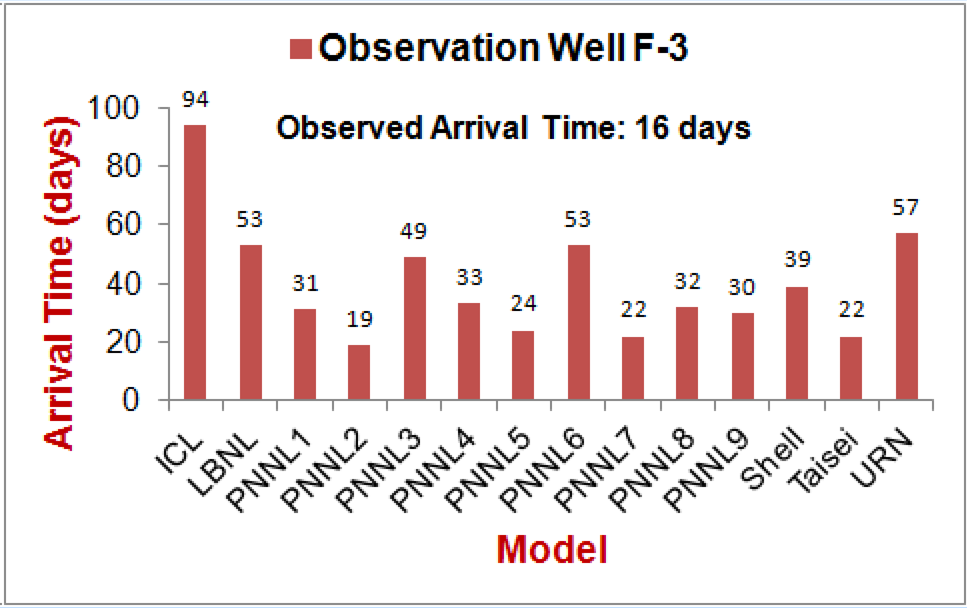
Location map of the S-3 site including the Detailed Area Study (DAS); Courtesy of JP Nicot



Task 3:

Sample Results from Model-to-Model Comparison





Task 3:
Interpretation Based on Statistical Analysis

Factors	F-2 Breakthrough Time, day	F-3 Breakthrough Time, day	Max Pressure 30d, MPa	Max Pressure 180d, MPa	Max Pressure 365d, MPa	RMSE bpw2, MPa	RMSE bpw3, MPa	RMSE MPa
Perm	*			***	**			*
Poro	**	*	***	****	**			
Perm to Poro	*			**	**			
R_{zx}	**		*	***	*	****		**
R_{zy}			**	**	*			
R_{yx}				**				
R_{zx}:R_{zy}				**	*		*	
Scheme	**	*	***	****	**	****	**	**

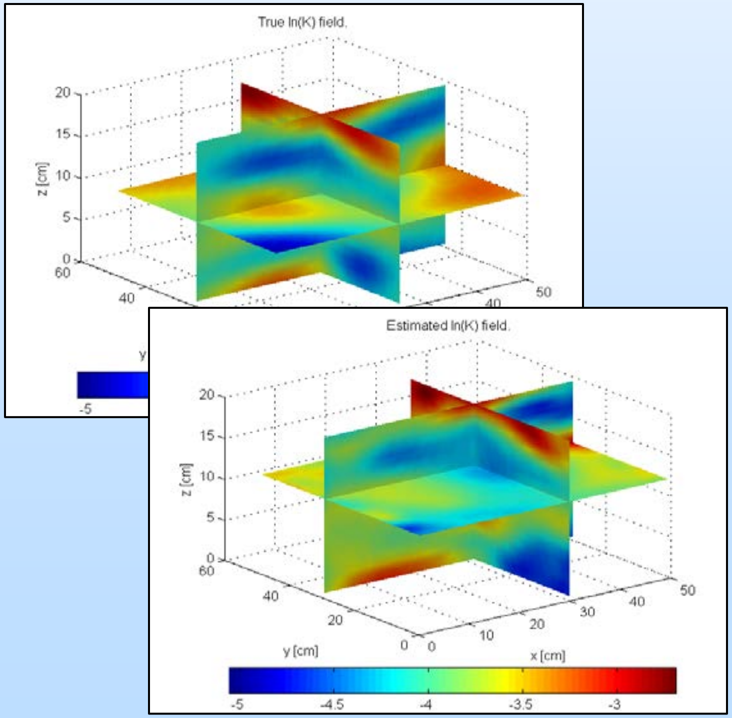
- Modeling scheme plays the most significant role
- Response variables are more sensitive to input parameters at intermediate times
- Simplified models (homogeneous and isotropic) produce the largest deviances
- Highly complex models (3-D heterogeneous and anisotropic) models have more simulation errors 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

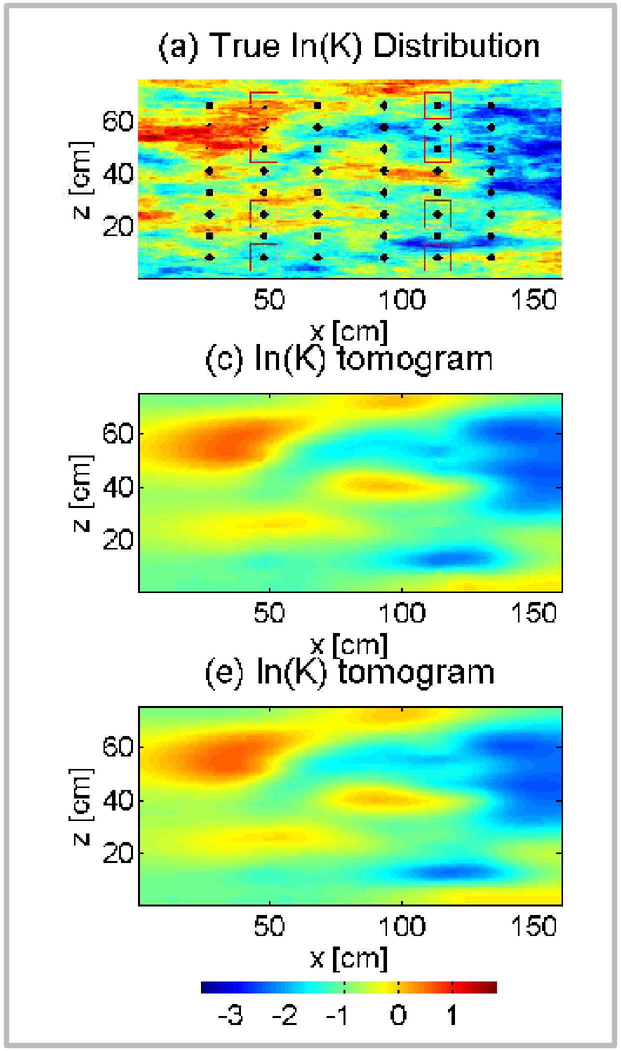
- **Objective**
  - Develop stochastic inversion methods as a superior calibration method for joint analysis of multiple types of uncertain and often very large data sets
  - Improve computational efficiency of existing inversion methods
  - Alleviate the computational hurdles associated with heterogeneity characterization and plume monitoring in field-scale CO_2 applications

- **Technical Status**
  - Introduced Krylov subspace methods to solve the geostatistical inversion system and designed efficient preconditioners
    - Avoids direct computing and storage of the sensitivity matrix
    - 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
    - Designed geostatistical reduced-order models (GROMs) for inverse problems with a large number of unknowns and a limited number of measurements
    - Reduced the size of the forward model by orders of magnitude

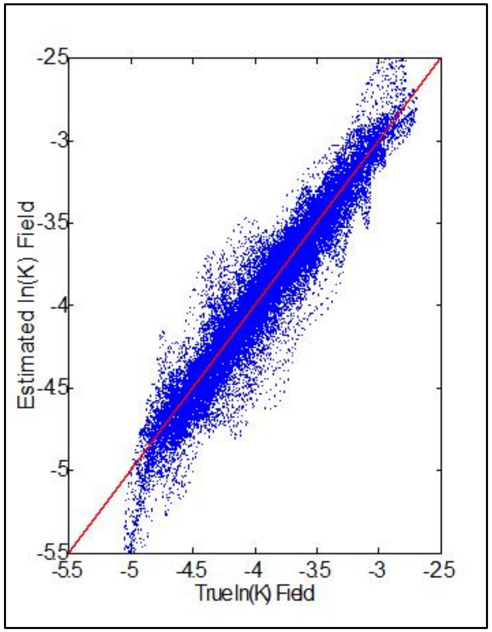


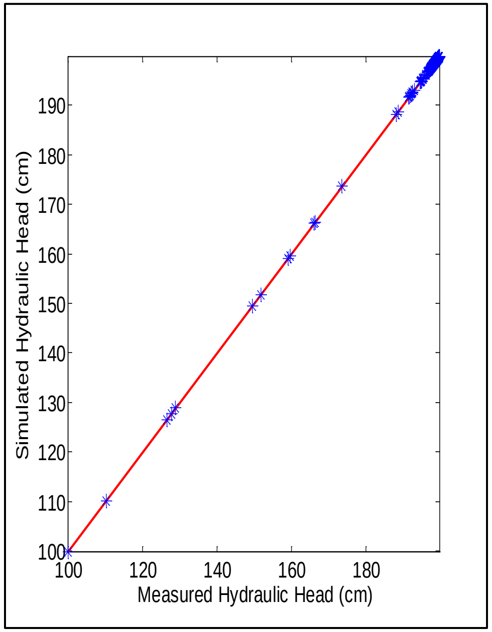
Task 4:

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 CO_2 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 CO_2 storage sites (e.g., using pumping test and CO_2 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 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: 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

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 pressure management
Marco Bianchi	Postdoctoral researcher	Supporting role in pressure management studies
Barbara Fialeix	Visiting graduate researcher	Supporting role in pressure management studies
Quanlin Zhou	PI and Research Scientist	Main scientist working on basin-scale simulations
Dorothee Rebscher	Project Scientist	Supporting role in basin-scale simulations
Sumit Mukhopadhyay	PI and Research Scientist	Main scientist working on Sim-SEQ
Xiaoyi Liu	Postdoctoral researcher	Main scientist working on stochastic inversion

Appendix: Gantt Chart for FY13

Task/Milestone (Fiscal Year / Quarter)	FY13 Q1	FY13 Q2	FY13 Q3	FY13 Q4
Task 1: Optimization of Brine Extraction for Pressure Management and Mitigation				
Incorporate Higher-Fidelity Simulators into the Optimization Framework	■			
Test Global Optimization Algorithms		■ I		
Apply IDPM Methodology to a Realistic Field Site			■	■ J
Task 2: Basin-scale Simulation of CO_2 Storage in the Northern Plains – Prairie Basal Aquifer				
Assess Dynamic Storage Capacity	■	■ G		
Assess Pressure Buildup and Environmental Impact for a Variety of Realistic Scenarios			■	■ H
Task 3: Sim-SEQ Model Comparison				
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	■	■ L		
Develop Model Reduction Methods for Improved Computational Efficiency			■	■
Methodology Demonstration Using Synthetic Data				■ M

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 CO_2 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

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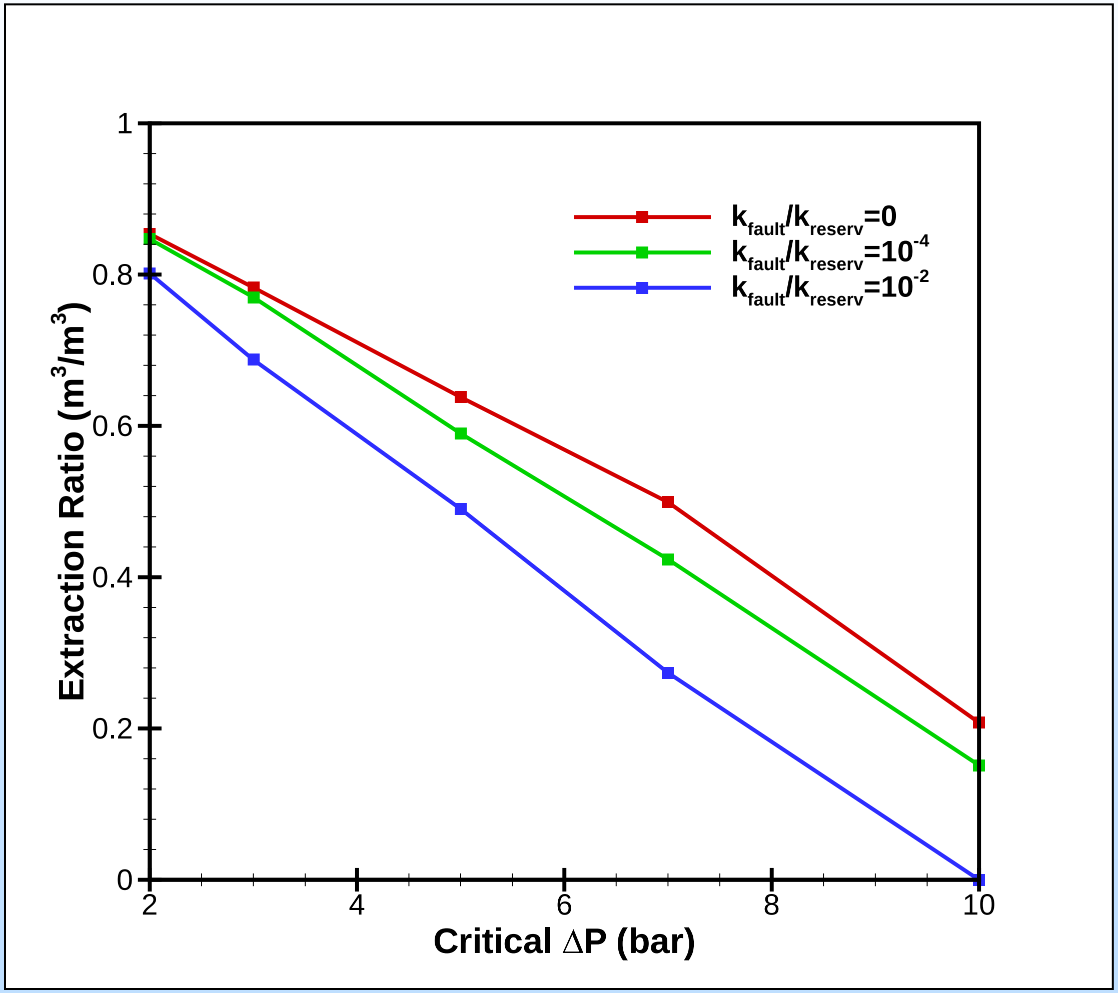
Backup

Task 1:

Effects of Critical Pressure and Fault Permeability on 'Extraction Ratio'



Extraction Ratio: Total Volume of Extracted Brine Divided by Injected CO_2