## Saline Formation GCS R&D Needs Workshop:

# Simulation

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# Definitions and Scope

- Modeling = mathematical and heuristic analyses (e.g., numerical and/or analytical solutions, curve fitting, interpolation, statistical methods) to predict or interpret the behavior of natural or engineered systems.
- Simulation = solving equations (e.g., numerical solutions to PDE's) that describe physical and other processes to predict or interpret the behavior of natural or engineered systems.
- Scope of consideration: Simulation of GCS in saline formations. Molecular dynamics and sub-pore-scale simulation are excluded.

# Purposes of Simulation

- Enhance characterization, estimate capacity
- Design injection and monitoring strategies
- Predict plume and pressure evolution
- Understand trapping mechanisms at diverse scales
- Manage and optimize injection and storage efficiency
- Interpret monitoring data, geophysical modeling
- History match by inverse modeling to refine properties
- Visualize and communicate injection processes
- Satisfy permitting and regulatory requirements
- Understand uncertainty and parameter sensitivity
- Contribute to risk assessment

# Current Status

- **Relatively mature area, used in every project**
- **Multiple respected codes are in use, active community**
- **Limitations and challenges exist**
  1. Data sparsity; proprietary data
  2. Size of problem (grid blocks, chemical components, …)
  3. Strength of coupling and number of coupled processes
  4. Simulating heterogeneity on diverse scales
  5. Simulating discrete features like fractures and faults
  6. Multiscale, multiphysics (e.g., pore to reservoir)
  7. Description and knowledge of processes (e.g., hysteretic $k_{rel}$)
  8. Scale-up of parameters from laboratory measurements
  9. Validation and verification
  10. Data input (e.g., from geomodel) and gridding
  11. Post-processing, interpreting, and analyzing results

# Simulation R&D is in Two Areas

## 1) Applications, e.g.,

- Very large-scale simulations (O($10^7$) grid blocks)
- Improved understanding of trapping mechanisms
- Reactive transport
- Pressure rise and dissipation
- Intercomparison studies

## 2) New capabilities, e.g.,

- THMC coupling
- Multiscale and multiphysics modeling
- Coupled systems (e.g., wellbore, atmosphere)
- Improved grid generation, data input, post-processing
- Fracturing and faulting

# Reiterate Scope

- Restrict consideration to simulation of reservoirs, cap rock, overburden, well bores, geophysics (continuum scale).
- Includes pore-scale to reservoir-scale models.
- Includes upscaling (pore-scale models developed in the lab upscaled to core, and core scale upscaled to reservoir).
- Includes geophysical simulation (e.g., propagation of seismic waves in multiphase porous medium)
- Includes inversion, as constrained by geophysical and hydrologic data and forward simulations.
- Includes geomechanical and geochemical simulation.

# Simulation Workflow

Simulator

- Choose system (fluids, domain, BC's, IC's)
- Choose processes including couplings
- Develop or assume model equations describing procs.
- Develop or adopt algorithms for solving model eqns.
- Implement (code) algorithms
- Verify the code (algorithms) over range of problems that includes problem(s) of interest
- Discretize the domain (gridding)
- Assign system properties and time, inj./prod., BC's, IC's
- Assign simulation parameters and run the code
- Analyze results

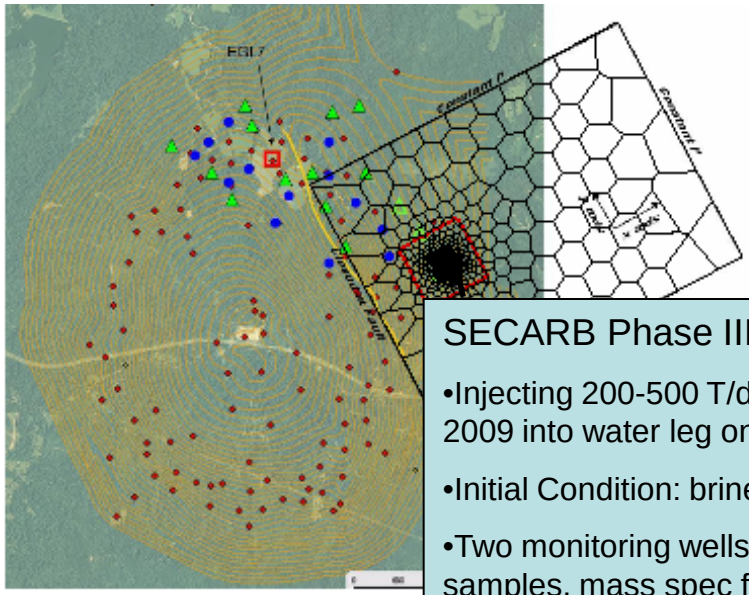
# Practical Aspects

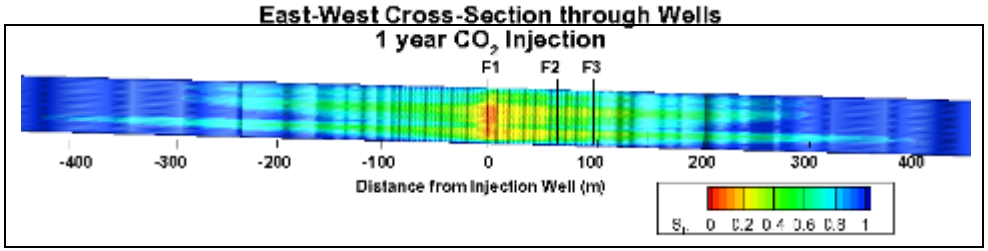
- Geomodel development
- Gridding
- Specification of input parameters
- Monitoring the computation itself
- Processing and interpreting output

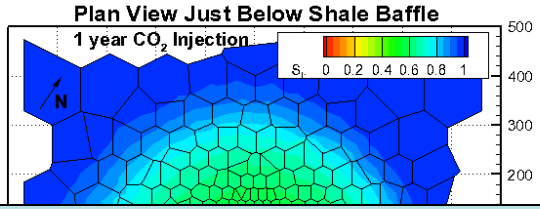
Some examples follow…

# GCS Pilot-Test Simulation (Chris Doughty (LBNL))

## Denbury $CO_2$-EOR at Cranfield, Mississippi  Model Results



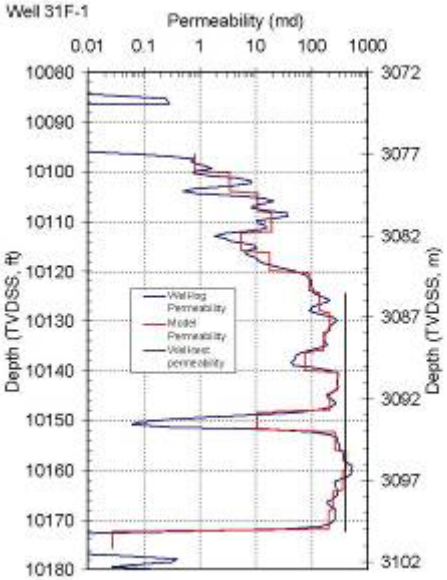




### SECARB Phase III $CO_2$ Injection

- Injecting 200-500 T/day $CO_2$ since December 2009 into water leg on flank of dome
- Initial Condition: brine saturated with $CH_4$
- Two monitoring wells with U-Tubes to collect samples, mass spec for gas composition
- Multiple tracer pulses released
- Time-lapse well logging for saturation profiles
- Seismic and electrical resistivity imaging

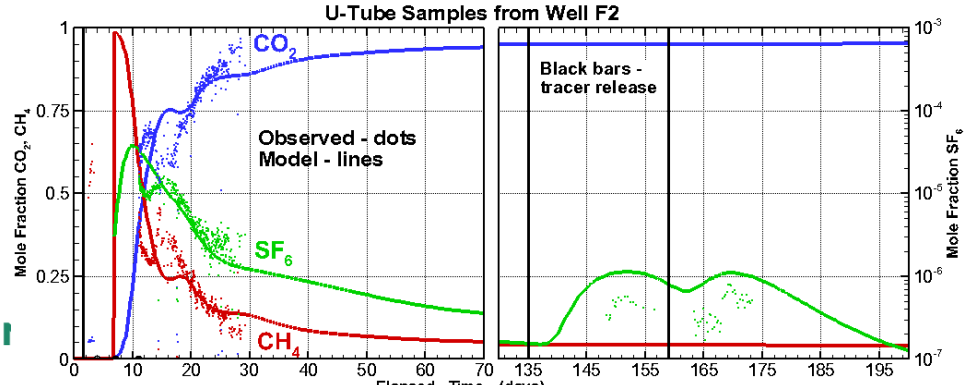
### Key Features in Breakthrough Curves

- Pulse of gas-phase $CH_4$ forms at leading edge of plume as $CO_2$ preferentially dissolves
- Multiple $CH_4$ peaks illustrate distinct flow paths above and below shale baffle
- Low, wide peaks for later tracer releases - evidence of self-sharpening plume front

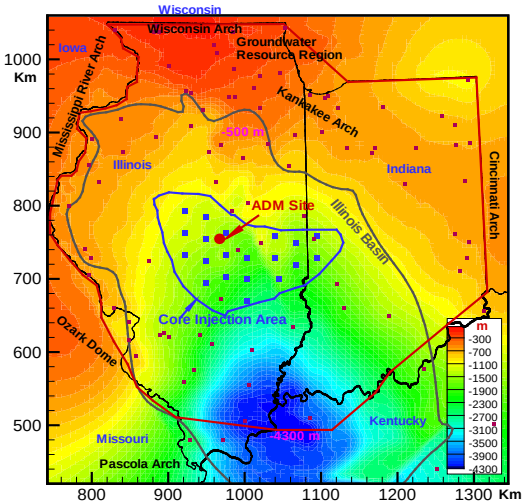



### Model Development

- Injection-well log shows two high-permeability layers separated by a shale baffle
- Layered model, finer at wells
- $CO_2$ injected over interval shown by black bar

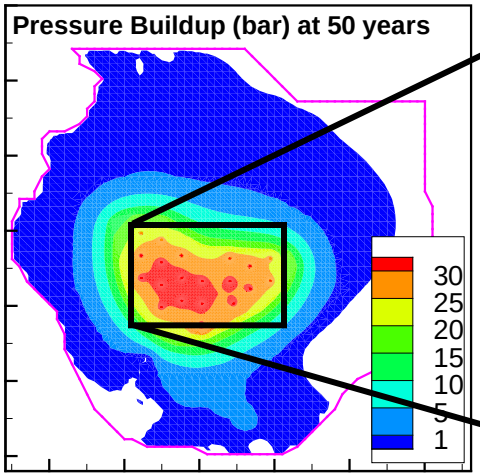


# Simulations of a Full Deployment $CO_2$ Storage Scenario in the Illinois Basin (Zhou and Birkholzer (LBNL))

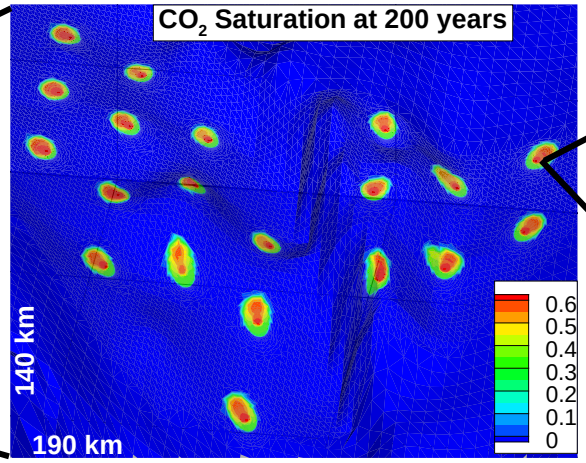



Elev. of the top of the Mt. Simon Fm.

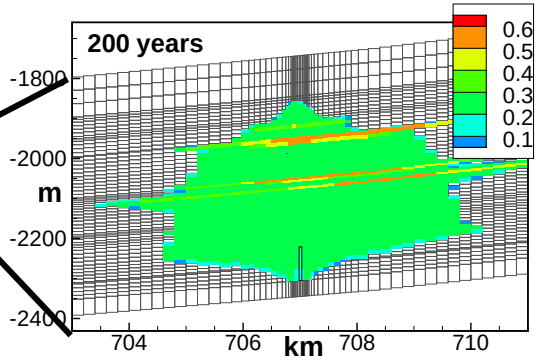
- Concern has been raised that $CO_2$ storage causes unacceptable pressure rise (e.g., Ehlig-Economides and Economides, J. Petrol. Tech., 2010).
- We have simulated the injection of 5 Gt $CO_2$ over 50 years at 20 sites (5 Mt/yr at each site) in the Mt. Simon Formation.
- Simulated pressure rise is approx. 30 bars centered in the injection area. This pressure dissipates with time as brine flows into low-permeability cap rock over large areas.
- $CO_2$ plumes from each of the 20 injection sites do not intermingle as 3D effects (vertical flows) allow efficient filling of pore space (Zhou and Birkholzer, GHGS&T, 2011).




Pressure rise (bar) at end of injection

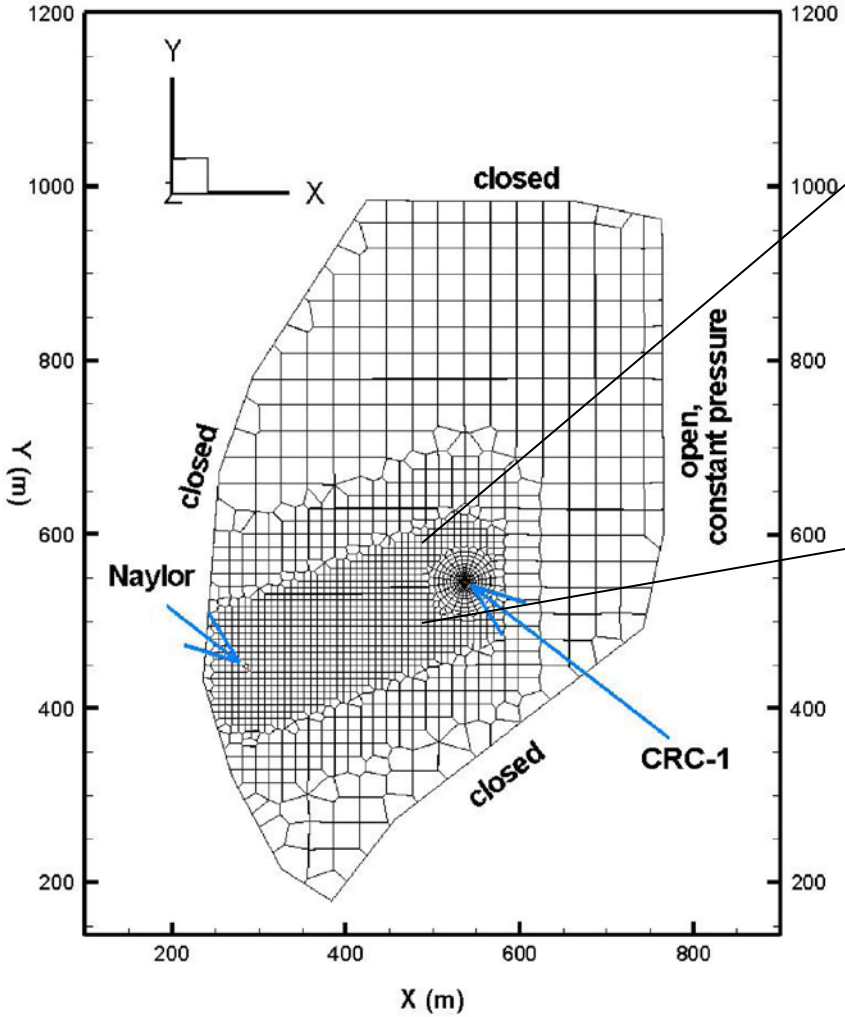


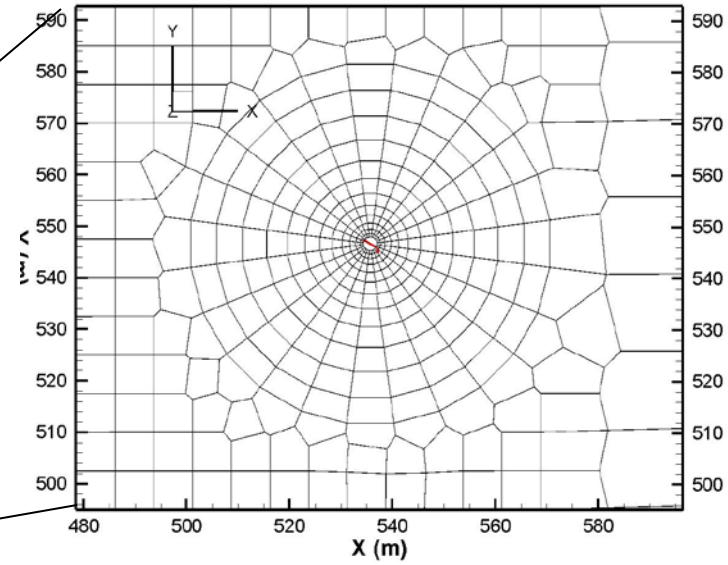

$CO_2$ saturation after 200 years

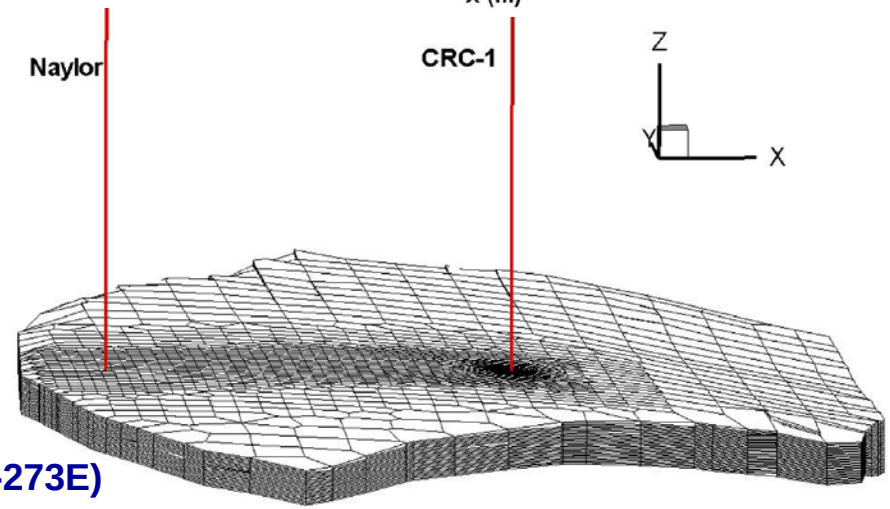



Vertical cross-section of $CO_2$ saturation after 200 years for one site.

# Gridding for Otway Phase 1



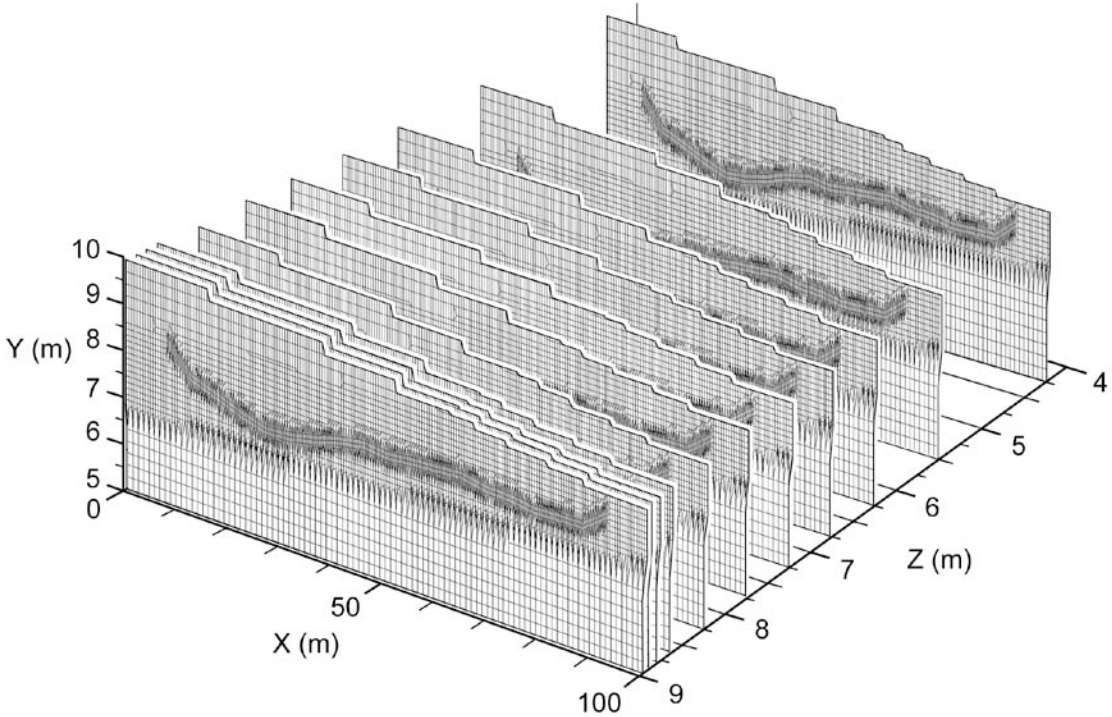




Gridding by Lehua Pan with Wingridder (LBNL-273E)

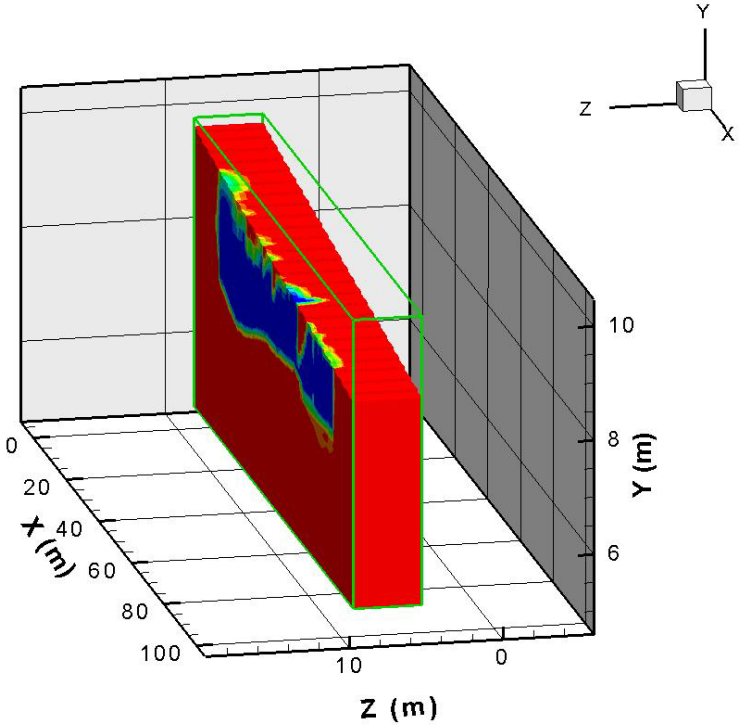
For Oldenburg, Pan, and Freifeld, unpublished 2009.

# ZERT Shallow-Release Simulation with TOUGH2/EOS7CA (Oldenburg et al.)

**Highly detailed grid emphasizes details of horizontal well (grid by Pan using Wingridder, LBNL-273E).**

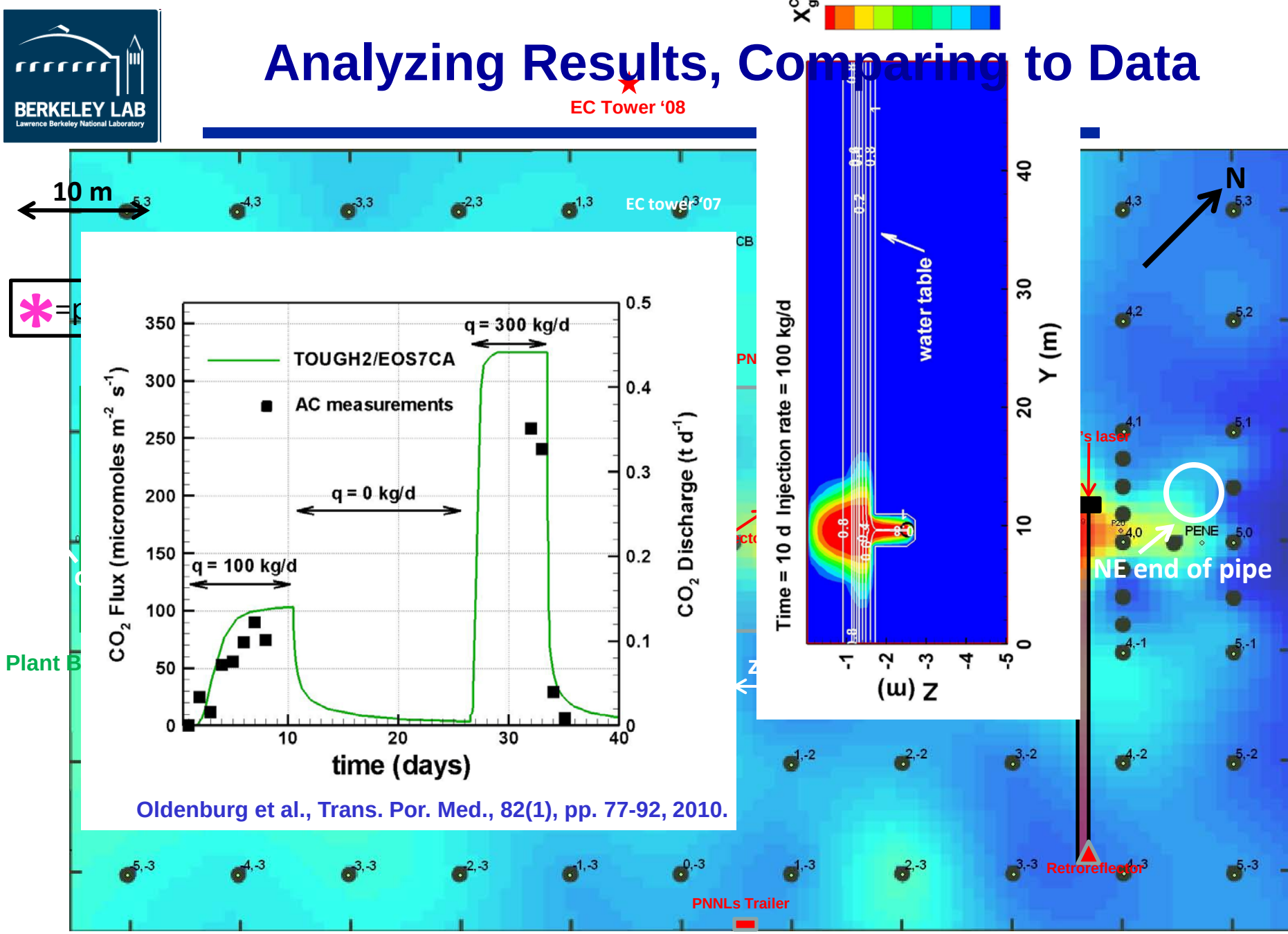



**Patchy emission pattern emerges as observed in the field.**




**Oldenburg et al., Env. Earth Sci., 60, 241-250, 2010.**

# Analyzing Results, Comparing to Data



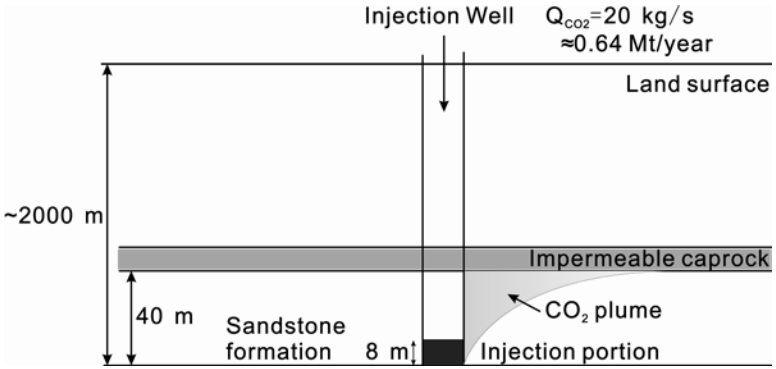

Oldenburg et al., Trans. Por. Med., 82(1), pp. 77-92, 2010.

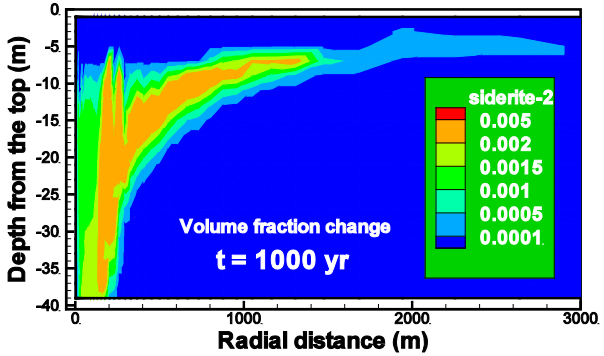
# GCS Reactive Transport Modeling (Tianfu Xu (LBNL))

## TOUGHREACT modeling of fate of injected $CO_2$ in three phases

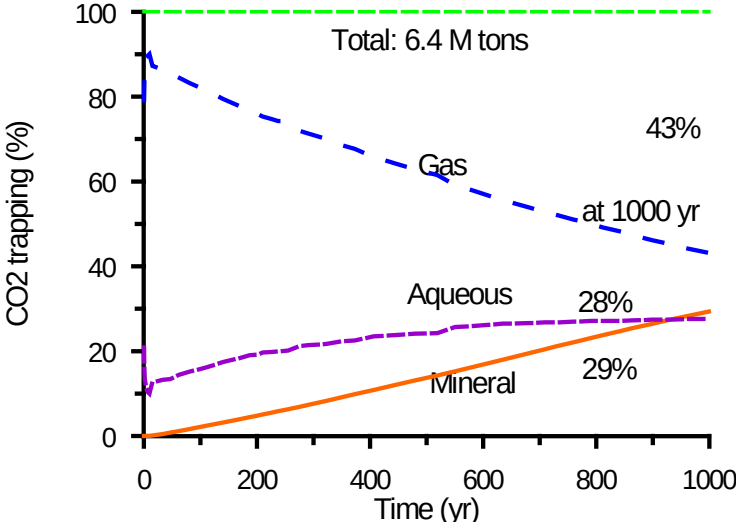
(Xu et al., Computers & Geosciences, 2011)

**A 2-D radial model for $CO_2$ injection into a sandstone formation using Gulf Coast mineralogy**



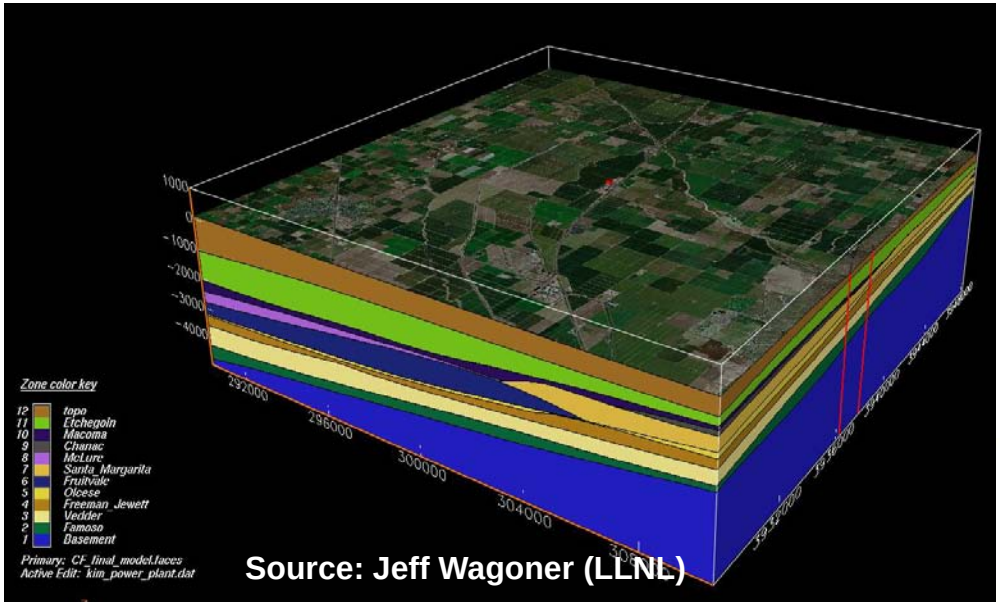




**Percentage of $CO_2$ sequestered in three phases over time.**



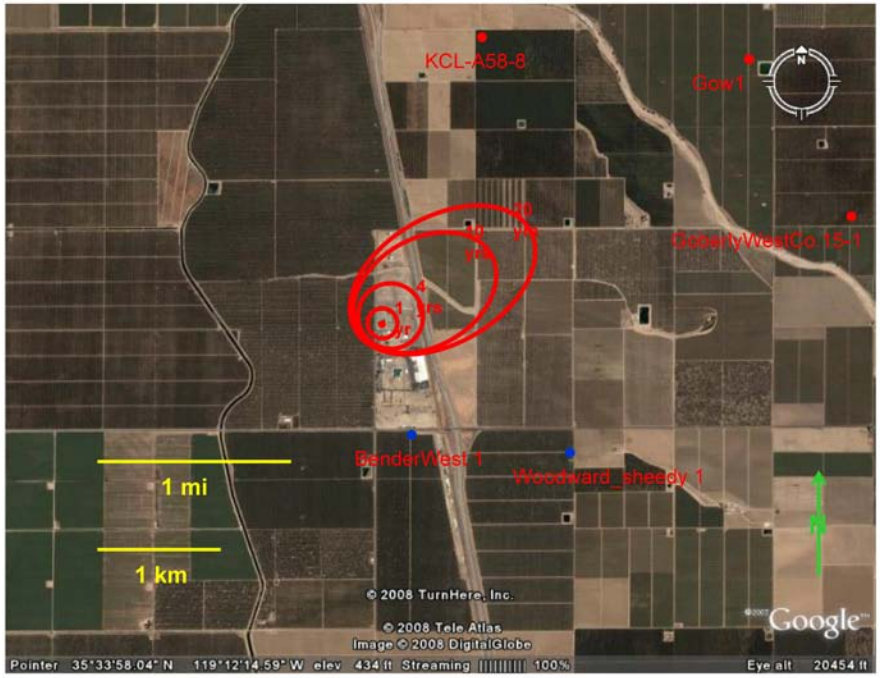

- **The mineral trapping starts at late stage (about 50 years) and then increases linearly with time.**
- **After 1,000 years, 29% of the injected $CO_2$ can be trapped in the solid (mineral) phase, 28% in the aqueous, and 43% in the gas phase.**

# Simulation to Understand Trapping (Chris Doughty (LBNL))




Source: Jeff Wagoner (LLNL)

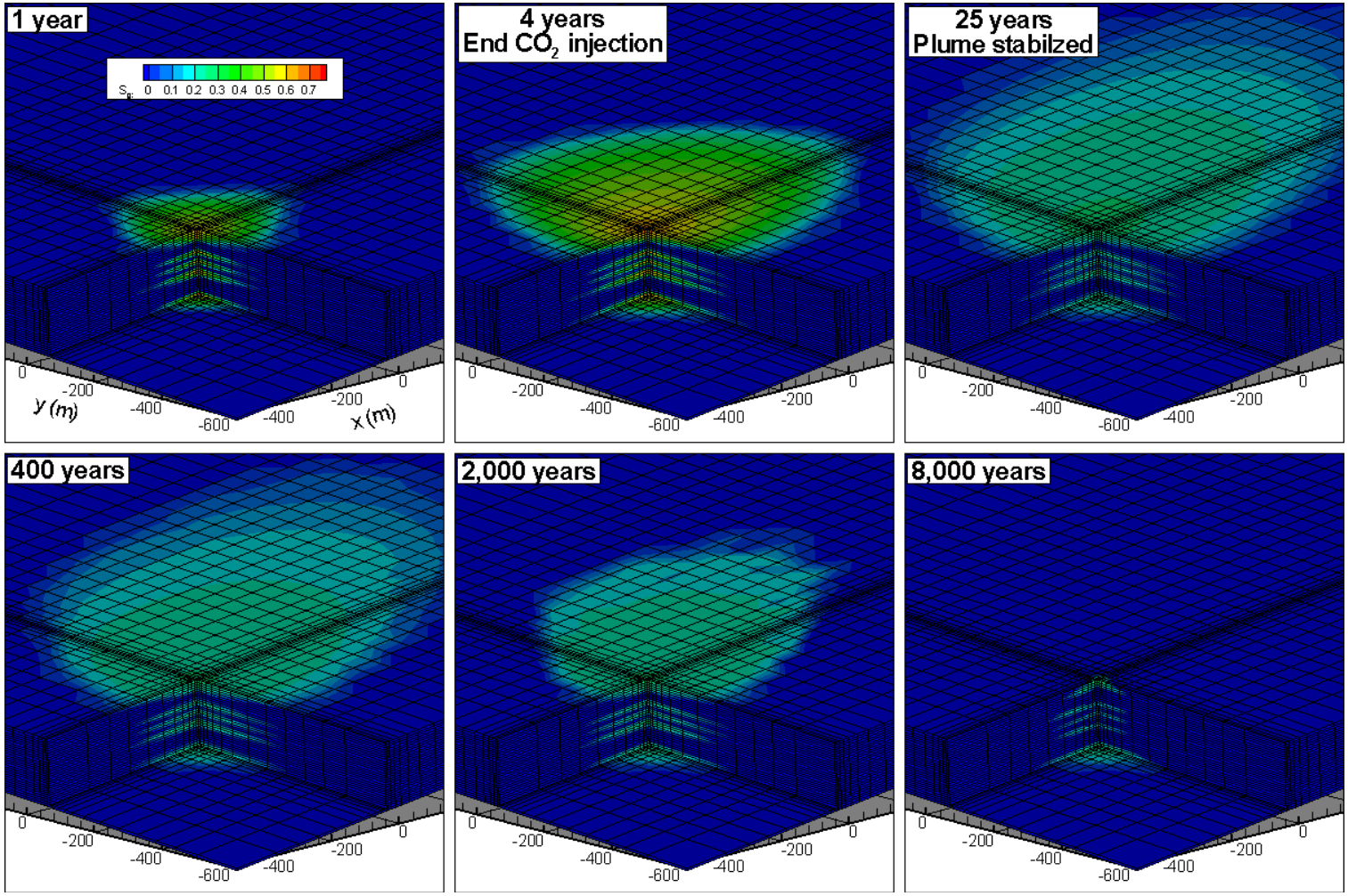
## Southern San Joaquin Valley




**250,000 t/yr for four years**

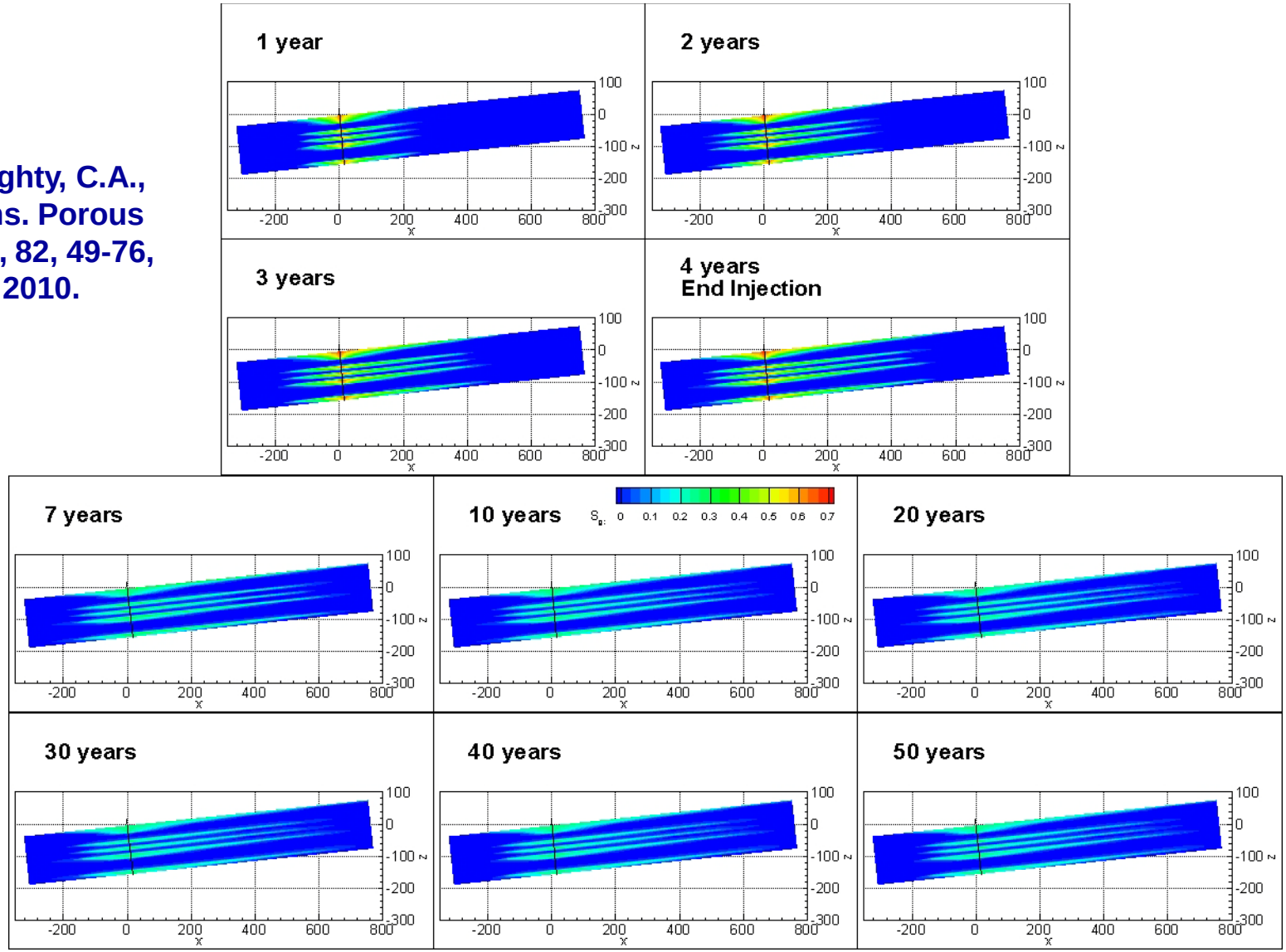
**TOUGH2 simulation of $CO_2$ plume.**

# Evolution of Plume

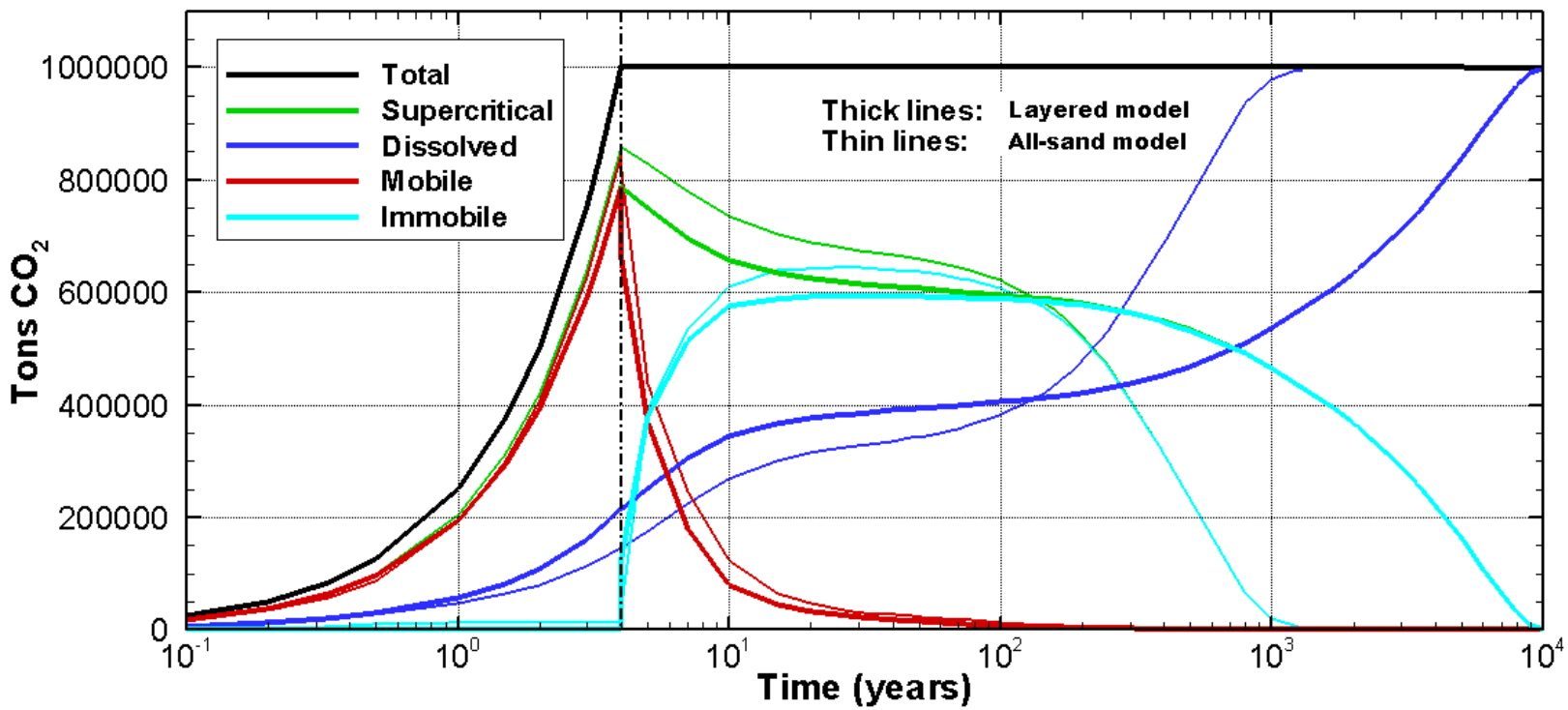


# Saturation in Cross Section

Doughty, C.A., Trans. Porous Med., 82, 49-76, 2010.



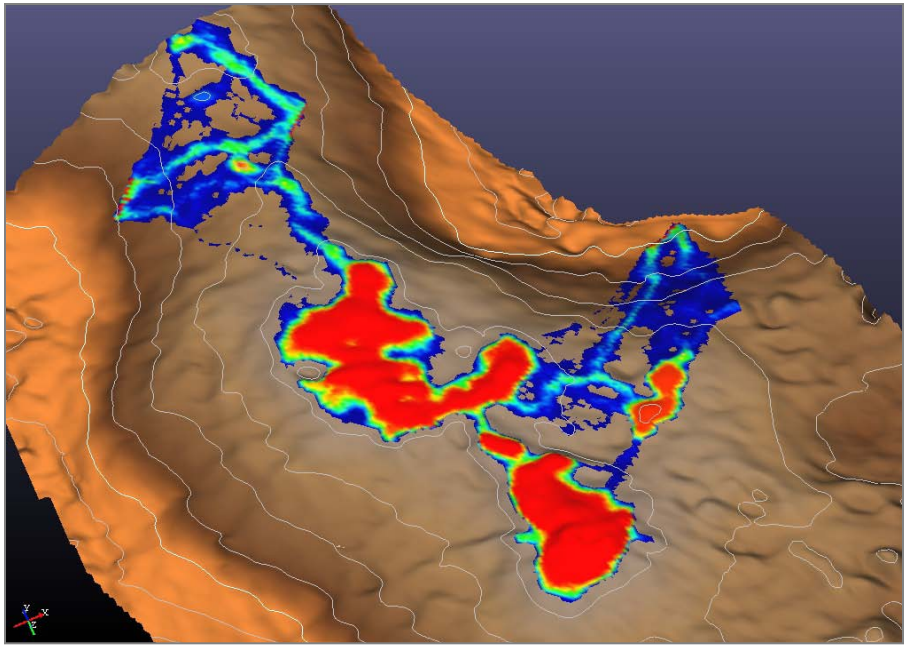
# $CO_2$ Inventory Evolution



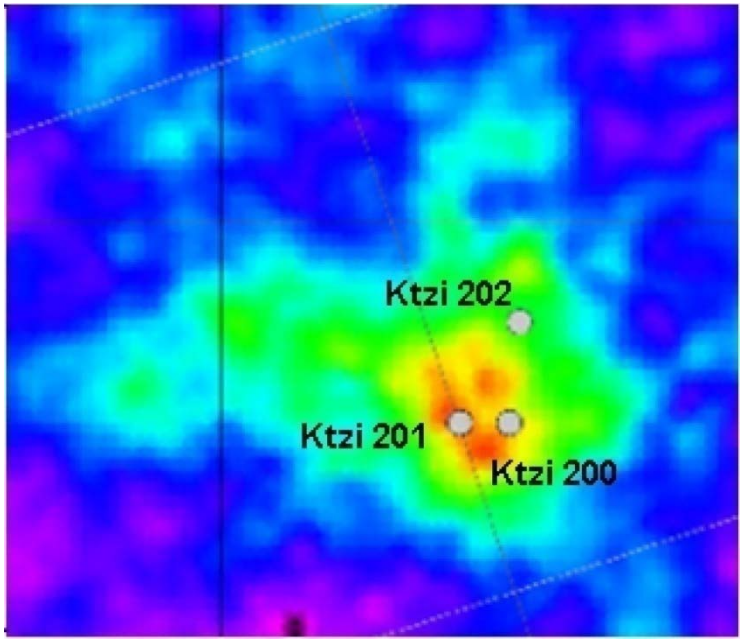

Doughty, C.A., Trans. Porous Med., 82, 49-76, 2010.

# Heterogeneity

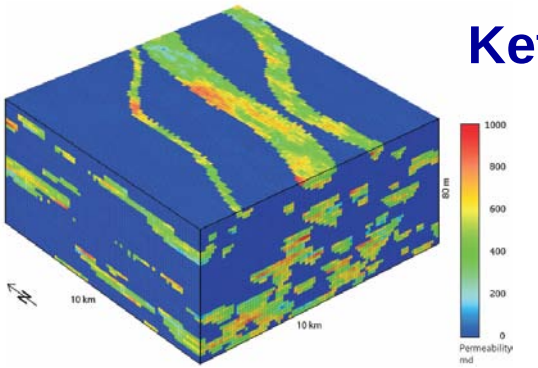
$CO_2$ Migration Beneath Caprock by Invasion Percolation simulation (Cavanagh et al., 2010)



**In Salah**




**Ketzin**




**(Bergmann et al., 2011)**

# Practical Needs

- Convenient translation of geomodel to numerical simulator input
- Gridding over diverse scales
- Ability to carry out very large problems addressing applications including scientific questions
- Carrying out multiple runs for uncertainty analysis or optimization or parameter sensitivity purposes
- Verification of results
- Interpreting results
- Communicating the results to others
- Developing simplified models that others can use

# Some Application R&D Needs (1)

- Better descriptions/models of system properties
  - Scaled-up parameters, multiscale heterogeneity
  - $P_{cap}$ and $k_r$ dependence on composition, swelling
  - High-salinity fluid properties
  - Pure and mixed-gas adsorption
  - Permeability as f(grain dissolution/precipitation)
- Better understanding of pressure evolution
- Better understanding of trapping mechanisms
- Better methods to interpret field observations and synthesize data for use in simulations, develop integrated conceptual models
- Protocols for verification, code comparison, modeling comparison

# Some Application R&D Needs (2)

- Improved estimation of reservoir parameters and processes through coupled inversion of time-lapse THMC-geophysical datasets
- Development of best practices, classification of sites, protocols or guidelines on how to model the different types of sites
- Joint validation study using a medium- to large-scale well-constrained system (e.g., large block, long column such as LUCI)
- Better understanding of heterogeneous fluid distributions and corresponding geophysical properties (e.g., seismic and electrical)

# Some Capability R&D Needs (1)

- Better gridding and geomodel-to-simulator tools
- Higher-speed computing for repeated sims. for UQ
- Practical (large enough) fully coupled models (parallelization needs for coupled systems).
- Multiscale and multiphysics (e.g., flow in pores and wells coupled to reservoir or cap rock)
- Ability to model induced seismicity (reactivation of faults) and fracturing with coupling to flow
- Higher-order schemes in space and time
- Reduced and simplified models for use by regulators and others

# New Directions?

- Community-based simulator(s)
- Public domain (non-proprietary) codes
- Toolbox approach rather than single application
- Web- and cloud-based simulation
- More generalization (less specialization)
- Simpler rather than more complex
-

# Conclusions

- Simulation is a relatively mature technology
- Significant improvements are needed to handle complexities of GCS
  - THMC coupling
  - Large-scale problems, e.g., to handle heterogeneity
  - Emphasis on UQ and parameter sensitivity
  - Property and behavior descriptions
  - Use and synthesis of field data
  - Coupling with geophysical monitoring and joint inversion
  - Multiscale and multiphysics simulation
- Reduced or simplified models are also needed

# Acknowledgments

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